STIC Search Report
Biotech-Chem Library

STIC Database Tracking Number: 122844

TO: Alton Pryor **Location:** **Art Unit: 1616** **May 24, 2004** **Case Serial Number: 09/666463**	**From: P. Sheppard** **Location: Remsen Building** **Phone: (571) 272-2529** **sheppard@uspto.gov**

HC 10

Search Notes

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=> fil hcaplus
FILE 'HCAPLUS' ENTERED AT 14:23:41 ON 24 MAY 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907 - 24 May 2004  VOL 140 ISS 22
FILE LAST UPDATED: 23 May 2004  (20040523/ED)

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

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=> d stat que l24
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L2               STR
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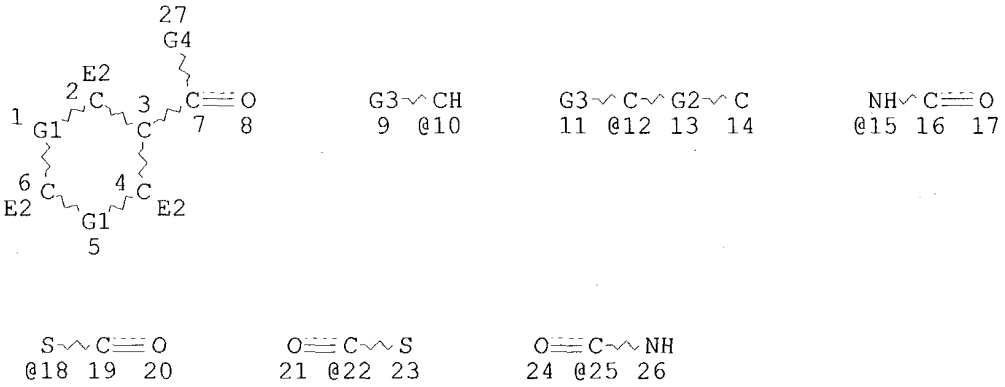


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REP G2=(0-5) C
VAR G3=15/18/22/25
VAR G4=NH/S
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HCOUNT  IS E2     AT   4
HCOUNT  IS E2     AT   6
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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NUMBER OF NODES IS  27

STEREO ATTRIBUTES: NONE
L4               STR
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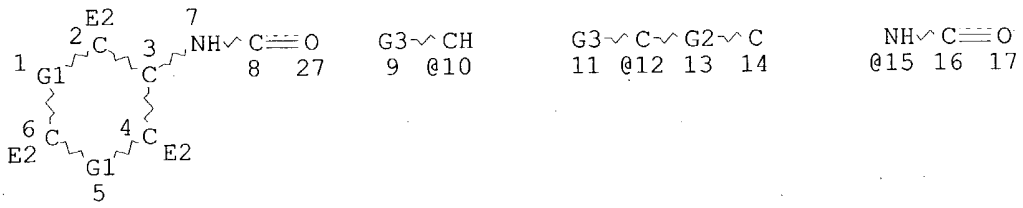

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REP G2=(0-5) C
VAR G3=15/18/22/25
NODE ATTRIBUTES:
HCOUNT IS E2 AT 2
HCOUNT IS E2 AT 4
HCOUNT IS E2 AT 6
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 27

STEREO ATTRIBUTES: NONE
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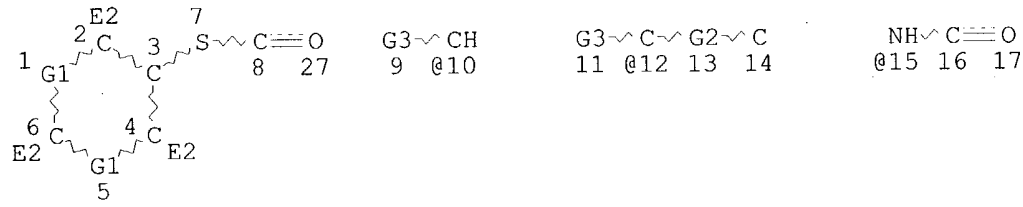

VAR G1=10/12
REP G2=(0-5) C
VAR G3=15/18/22/25
NODE ATTRIBUTES:
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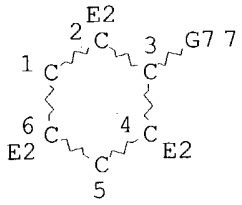
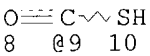
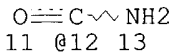
HCOUNT IS E2 AT 4
HCOUNT IS E2 AT 6
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

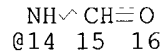
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 27

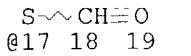
STEREO ATTRIBUTES: NONE
L8 142 SEA FILE=REGISTRY SUB=L1 SSS FUL L2 OR L4 OR L5
L11 STR

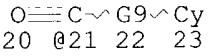


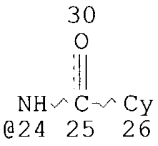


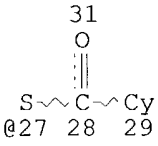








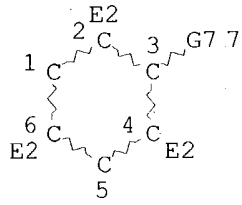


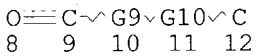


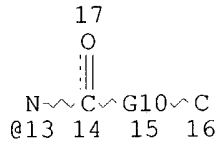
VAR G7=9/12/14/17/21/24/27
VAR G9=S/NH
NODE ATTRIBUTES:
HCOUNT IS E2 AT 2
HCOUNT IS E2 AT 4
HCOUNT IS E2 AT 6
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

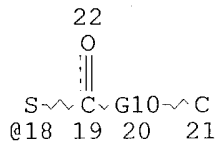
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 31

STEREO ATTRIBUTES: NONE
L14 11 SEA FILE=REGISTRY SUB=L8 SSS FUL L11
L17 STR









VAR G7=9/13/18
VAR G9=S/NH
REP G10=(0-20) C
NODE ATTRIBUTES:
HCOUNT IS E2 AT 2
HCOUNT IS E2 AT 4
HCOUNT IS E2 AT 6
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 22

STEREO ATTRIBUTES: NONE

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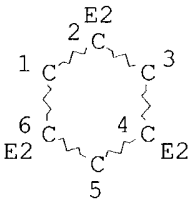
L20 130 SEA FILE=REGISTRY ABB=ON PLU=ON L19 OR L14
L22 STR



VAR G1=7/9
NODE ATTRIBUTES:
HCOUNT IS E2 AT 2
HCOUNT IS E2 AT 4
HCOUNT IS E2 AT 6
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 11

STEREO ATTRIBUTES: NONE
L23 12 SEA FILE=REGISTRY SUB=L20 SSS FUL L22
L24 2 SEA FILE=HCAPLUS ABB=ON PLU=ON L23

=> d ibib abs hitstr 1-2

L24 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:929374 HCAPLUS
DOCUMENT NUMBER: 139:396167
TITLE: Preparation of amino acid derivatives as gelling agents
INVENTOR(S): Van Bommel, Kjeld Jacobus Cornelis; Van Esch, Johannes Henricus; De Loos, Maaike; Heeres, Andre; Feringa, Bernard Lucas
PATENT ASSIGNEE(S): Applied Nanosystems B. V., Neth.
SOURCE: Eur. Pat. Appl., 17 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1364941	A1	20031126	EP 2002-77007	20020522
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
WO 2003097587	A2	20031127	WO 2003-NL381	20030522
WO 2003097587	A3	20040311		
W: AE, AG, AL, AM, AT, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EC, EE, EE, ES, FI, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC,				

NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: EP 2002-77007 A 20020522

OTHER SOURCE(S): MARPAT 139:396167

AB The invention relates to a novel class of gelling agents Y1n-Am1-X1-Z(-X2-Am2-Y2n)(-X3-Am3-Y3n) [Z is (hetero)cycloalkyl or (hetero)aryl; X1, X2, X3 are NH, CO, or NHCO; Am1, Am2, Am3 are amino acids or derivs. or a no. of amino acids or derivs.; Y1, Y2, Y3 are OH, OR, NHR, where R is (cyclo)alk(en)(yn)yl; n = 1 or 2 (with provisos)] and to a process for their prepn. Thus, Z-[Phe-O(CH2)7CH:CH2]3 (Z is cis,cis-1,3,5-cyclohexanetricarbonyl) was prepd. via amidation reaction and used to form a gel of Grubbs catalyst in benzene.

IT **627093-39-4**

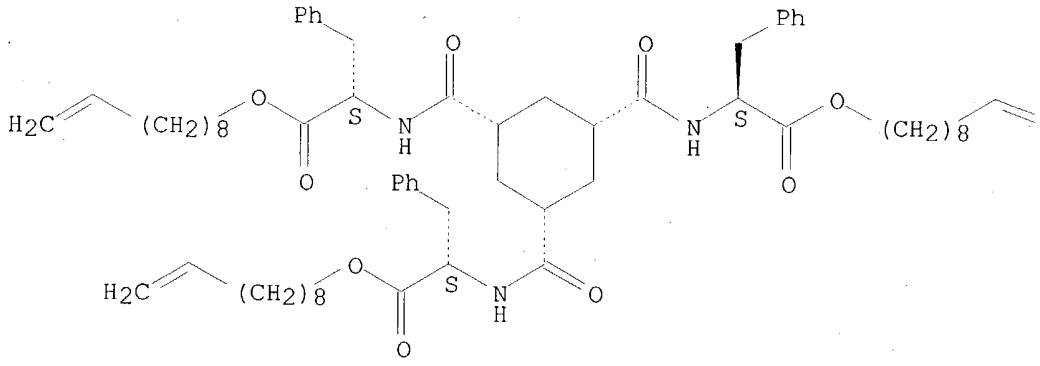
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(prepn. of amino acid derivs. as gelling agents)

RN 627093-39-4 HCAPLUS

CN L-Phenylalanine, N,N',N''-[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-cyclohexanetriyltricarbonyl]tris-, tri-9-decenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

$=CH_2$

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:225289 HCAPLUS

DOCUMENT NUMBER: 134:256618

TITLE: Cosmetic composition containing a cyclohexane derivative

INVENTOR(S): Livoreil, Aude

PATENT ASSIGNEE(S): L'Oreal, Fr.

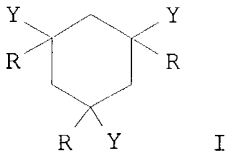
SOURCE: Eur. Pat. Appl., 13 pp.
CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1086945	A1	20010328	EP 2000-402369	20000828
EP 1086945	B1	20021009		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
FR 2798655	A1	20010323	FR 1999-11773	19990921
FR 2798655	B1	20011116		
AT 225766	E	20021015	AT 2000-402369	20000828
ES 2184686	T3	20030416	ES 2000-402369	20000828
JP 2001114630	A2	20010424	JP 2000-287797	20000921

PRIORITY APPLN. INFO.: FR 1999-11773 A 19990921
OTHER SOURCE(S): MARPAT 134:256618
GI



I

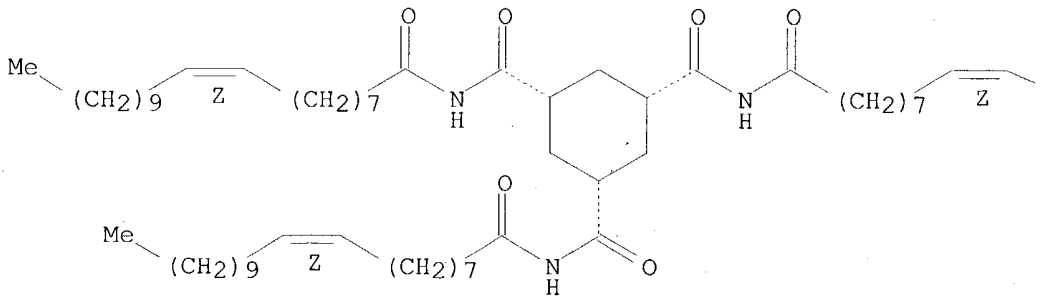
AB A cosmetic compn. contg. a cyclohexane deriv. [I; R = H, satd. hydrocarbon; Y = COSR', CONHR', NHCOR', SCOR' (R' = H, an aryl group substituted with a hydrocarbon chain)]. Thus, cis-1,3,5-tris(oleylaminocarbonyl)cyclohexane (II) was prepd. by the reaction of cis 1,3,5-cyclohexane-tricarboxylic acid with oleylamine. A cosmetic stick contained II 20.8, iron oxide 0.5 g, isododecane 16, and parleam oil 4 mL.

IT **330974-83-9 330974-84-0 330974-85-1 330974-86-2 330974-87-3 330974-88-4 330974-89-5 330974-90-8 330974-91-9 330974-92-0**
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
(cosmetic compn. contg. cyclohexane deriv.)

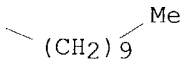
RN 330974-83-9 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris[(9Z)-1-oxo-9-eicosenyl]-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.

PAGE 1-A



PAGE 1-B



RN 330974-84-0 HCAPLUS
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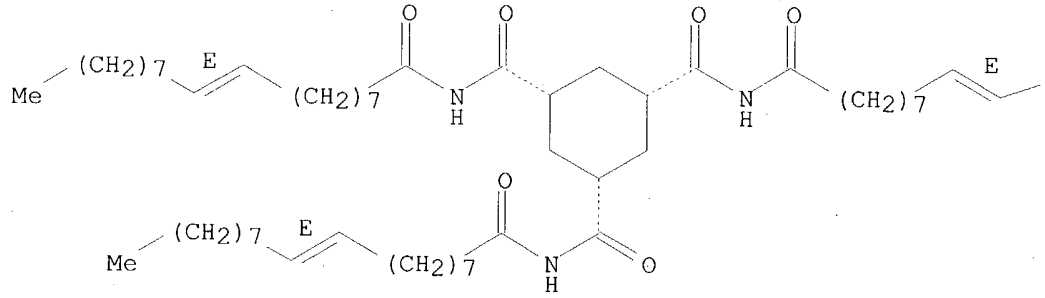
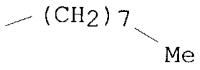
Relative stereochemistry.
Double bond geometry as shown.

PAGE 1-A



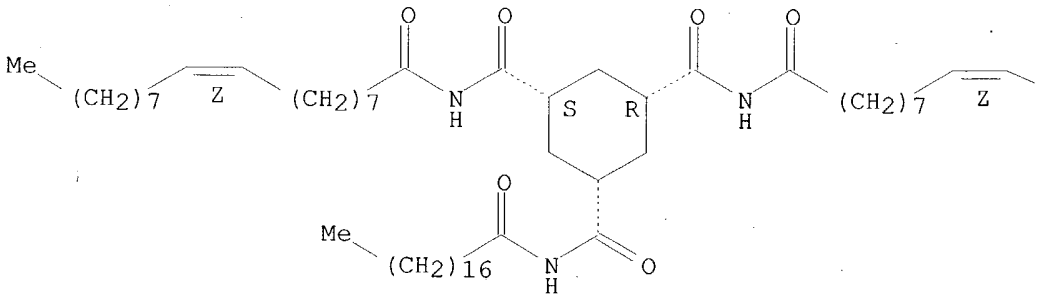
PAGE 1-B



RN 330974-85-1 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N'-bis[(9Z)-1-oxo-9-octadecenyl]-N''-(1-oxooctadecyl)-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.

PAGE 1-A



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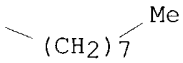
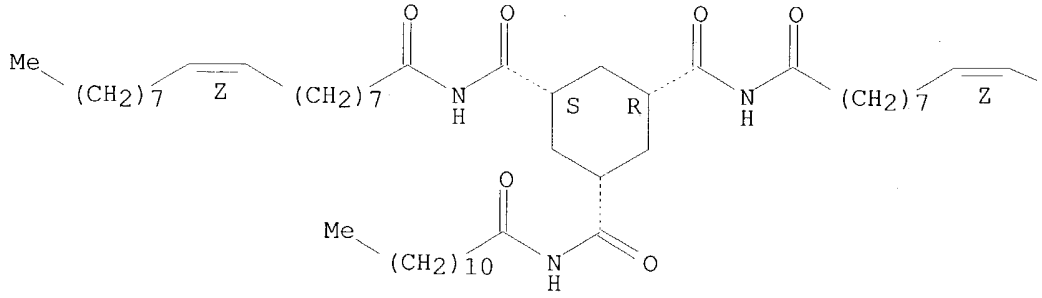


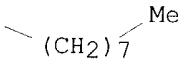
RN 330974-86-2 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N-(1-oxododecyl)-N',N''-bis[(9Z)-1-oxo-9-octadecenyl]-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.

PAGE 1-A



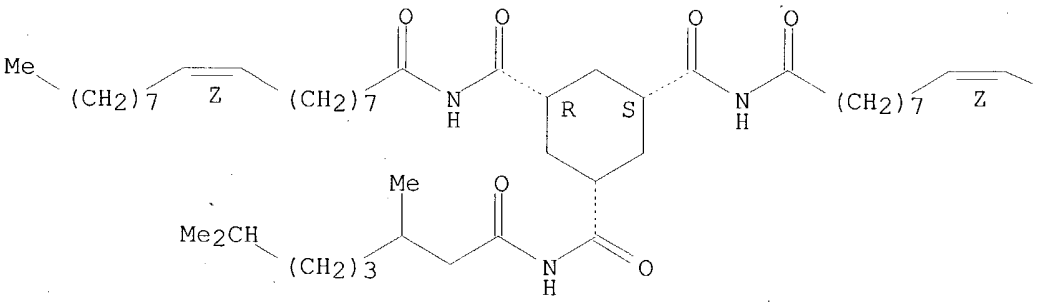
PAGE 1-B

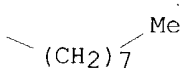


RN 330974-87-3 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N-(3,7-dimethyl-1-oxooctyl)-N',N''-bis[(9Z)-1-oxo-9-octadecenyl]-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.

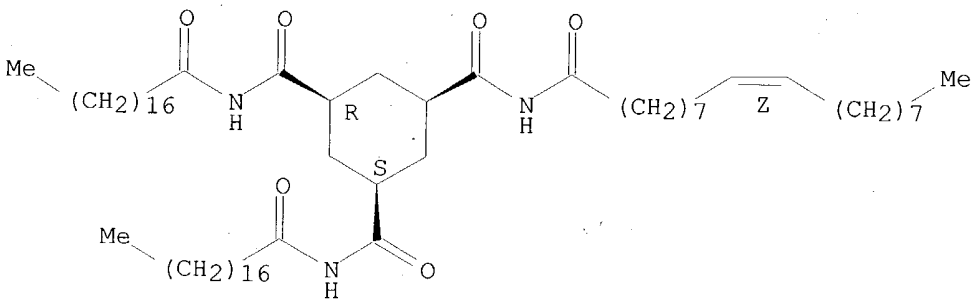
PAGE 1-A





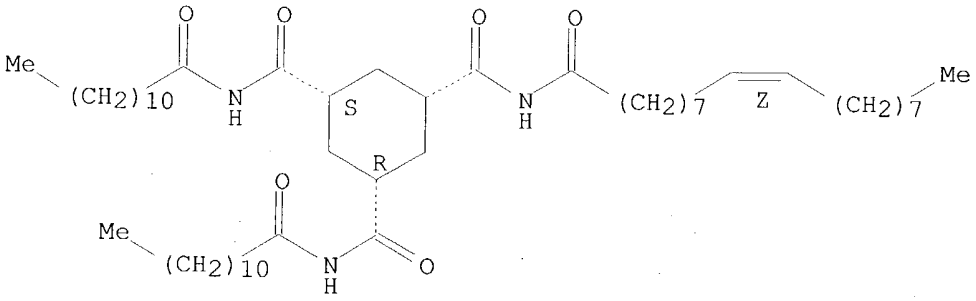
RN 330974-88-4 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N-[(9Z)-1-oxo-9-octadecenyl]-N',N''-bis(1-oxooctadecyl)-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



RN 330974-89-5 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N'-bis(1-oxododecyl)-N''-[(9Z)-1-oxo-9-octadecenyl]-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

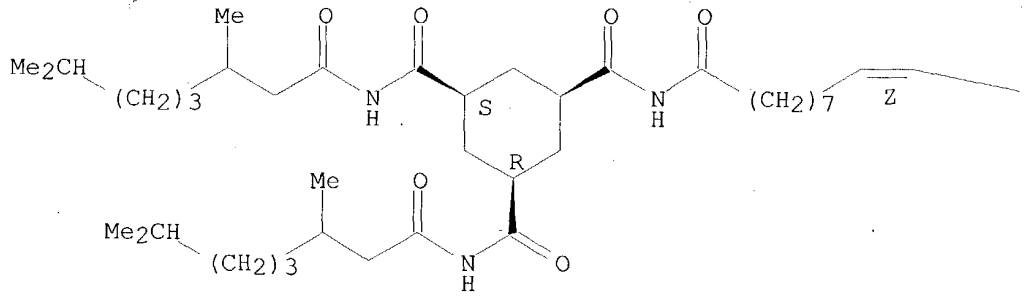
Relative stereochemistry.
Double bond geometry as shown.



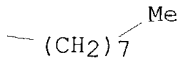
RN 330974-90-8 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N'-bis(3,7-dimethyl-1-oxooctyl)-N''-[(9Z)-1-oxo-9-octadecenyl]-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.

PAGE 1-A



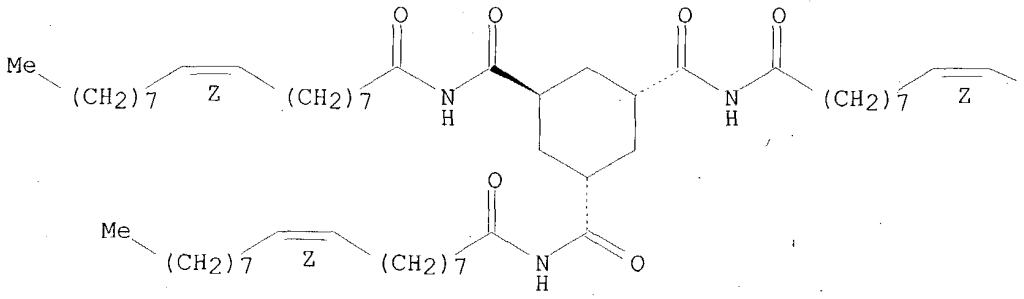
PAGE 1-B



RN 330974-91-9 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris[(9Z)-1-oxo-9-octadecenyl]-, (1.alpha.,3.alpha.,5.beta.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.

PAGE 1-A



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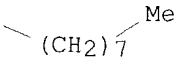

RN 330974-92-0 HCAPLUS
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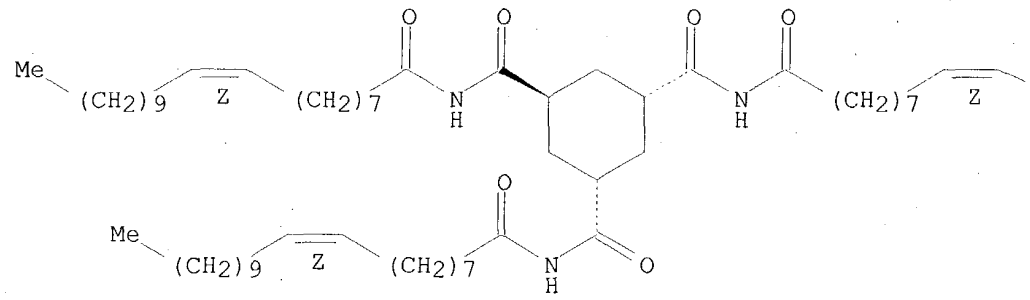
Relative stereochemistry.
Double bond geometry as shown.

PAGE 1-A



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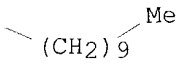
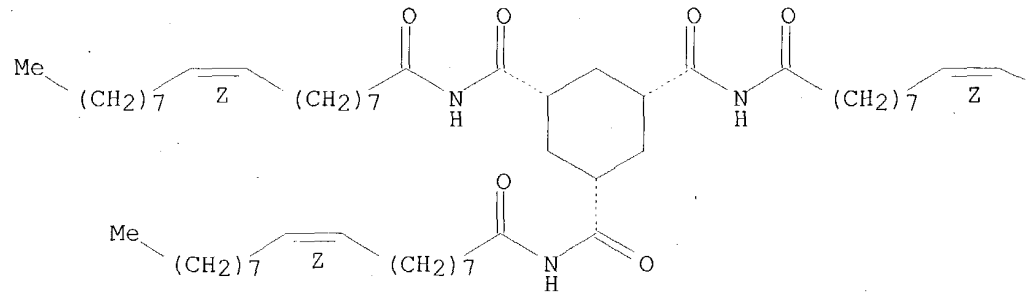


IT **330974-79-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(cosmetic compn. contg. cyclohexane deriv.)
RN 330974-79-3 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris[(9Z)-1-oxo-9-octadecenyl]-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.

PAGE 1-A



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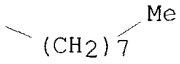

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L2               STR
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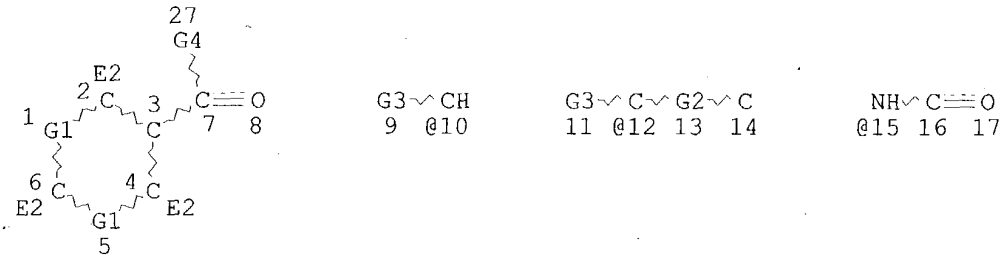


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REP G2=(0-5) C
VAR G3=15/18/22/25
VAR G4=NH/S
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HCOUNT  IS E2     AT   4
HCOUNT  IS E2     AT   6
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  27

STEREO ATTRIBUTES: NONE
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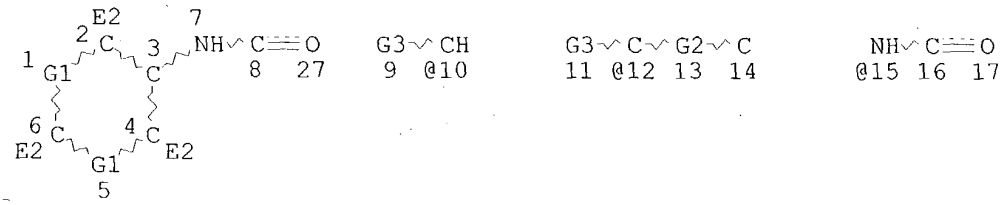

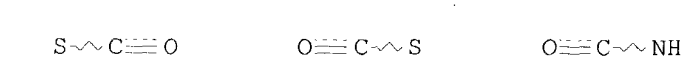


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VAR G1=10/12
REP G2=(0-5) C
VAR G3=15/18/22/25
NODE ATTRIBUTES:
HCOUNT  IS E2     AT   2
HCOUNT  IS E2     AT   4
HCOUNT  IS E2     AT   6
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
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NUMBER OF NODES IS 27

STEREO ATTRIBUTES: NONE
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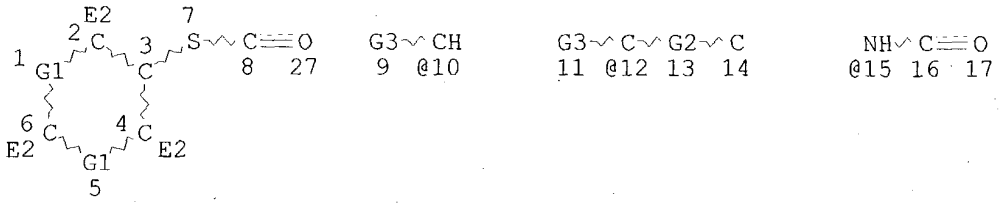

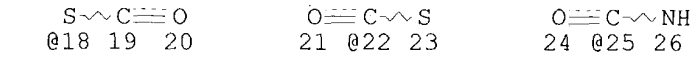

VAR G1=10/12
REP G2=(0-5) C
VAR G3=15/18/22/25
NODE ATTRIBUTES:
HCOUNT IS E2 AT 2
HCOUNT IS E2 AT 4
HCOUNT IS E2 AT 6
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 27

STEREO ATTRIBUTES: NONE
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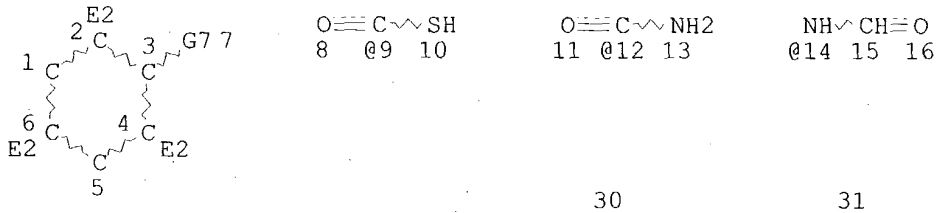

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VAR G9=S/NH
NODE ATTRIBUTES:
HCOUNT IS E2 AT 2
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HCOUNT IS E2 AT 6
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 31

STEREO ATTRIBUTES: NONE

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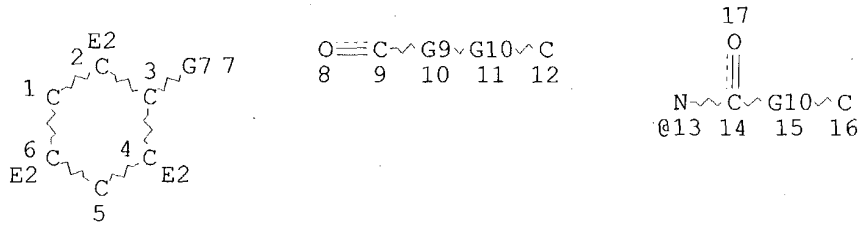
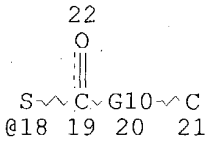
L17 STR





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VAR G9=S/NH
REP G10=(0-20) C
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HCOUNT IS E2 AT 4
HCOUNT IS E2 AT 6
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 22

STEREO ATTRIBUTES: NONE
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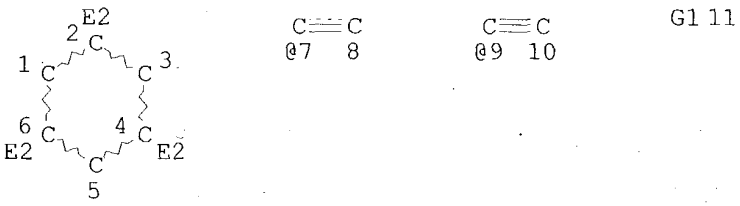
L22 STR



VAR G1=7/9
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HCOUNT IS E2 AT 2
HCOUNT IS E2 AT 4
HCOUNT IS E2 AT 6
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 11

STEREO ATTRIBUTES: NONE
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L24 2 SEA FILE=HCAPLUS ABB=ON PLU=ON L23
L25 118 SEA FILE=REGISTRY ABB=ON PLU=ON L20 NOT L23
L26 59 SEA FILE=HCAPLUS ABB=ON PLU=ON L25

L27 57 SEA FILE=HCAPLUS ABB=ON PLU=ON L26 NOT L24

=>
=>

=> d ibib abs hitstr l27 1-57

L27 ANSWER 1 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2004:203152 HCAPLUS
DOCUMENT NUMBER: 140:258619
TITLE: Cosmetic composition containing oils, a rheological agent and a particulate phase
INVENTOR(S): Blin, Xavier; Ferrari, Veronique
PATENT ASSIGNEE(S): L'Oreal, Fr.
SOURCE: Fr. Demande, 21 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2844186	A1	20040312	FR 2002-11095	20020906
EP 1405625	A1	20040407	EP 2003-20174	20030905

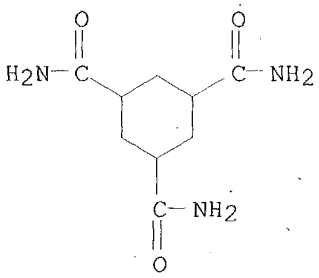
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK

PRIORITY APPLN. INFO.: FR 2002-11095 A 20020906

AB A cosmetic compn. comprises in a physiol. acceptable medium, at least a Ph silicone oil of high viscosity, at least a nonvolatile hydrocarbon oil having a mol. wt. higher than 500 g/Mol and/or an index of refraction at 20.degree.C higher than 1.440, at least a rheol. agent and a particulate phase. The compn. has good brightness, and comfort. A lipstick contained di-isostearyl malate q.s. 100, Ph trimethyltrisiloxane (20 cSt) (Dow Corning DC556) 18, Ph tri-Me trisiloxane (1000 cSt) (Belsil PDM 1000) 27, microcryst. wax 10, C30-45 alkyl dimethicone 2.5, a mixt. of lauric, myristic, palmitic, and stearic acid triglycerides, (50/20/10/10) (Softisan 100) 10, Red 7 0.26, Red 21, 0.06 black iron oxide 0.09, brown iron oxide 2,1 mica titanium oxide 1.8%.

IT **99063-92-0**, 1,3,5-Cyclohexanetricarboxamide
RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)
(cosmetic compn. contg. oils, rheol. agent and particulate phase)

RN 99063-92-0 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide (6CI, 9CI) (CA INDEX NAME)

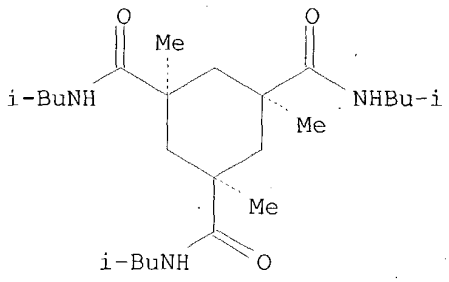


REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 2 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2003:1011634 HCAPLUS
DOCUMENT NUMBER: 140:163833
TITLE: Design, Synthesis, and in Vitro Biological Evaluation of Small Molecule Inhibitors of Estrogen Receptor .alpha. Coactivator Binding
AUTHOR(S): Rodriguez, Alice L.; Tamrazi, Anobel; Collins, Margaret L.; Katzenellenbogen, John A.
CORPORATE SOURCE: Department of Chemistry, University of Illinois, Urbana, IL, 61801, USA
SOURCE: Journal of Medicinal Chemistry (2004), 47(3), 600-611
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Nuclear receptors (NRs) complexed with agonist ligands activate transcription by recruiting coactivator protein complexes. In principle, one should be able to inhibit the transcriptional activity of the NRs by blocking this transcriptionally crit. receptor-coactivator interaction directly, using an appropriately designed coactivator binding inhibitor (CBI). To guide our design of various classes of CBIs, we have used the crystal structure of an agonist-bound estrogen receptor (ER) ligand binding domain (LBD) complexed with a coactivator peptide contg. the LXXLL signature motif bound to a hydrophobic groove on the surface of the LBD. One set of CBIs, based on an outside-in design approach, has various heterocyclic cores (triazenes, pyrimidines, trithianes, cyclohexanes) that mimic the tether sites of the three leucines on the peptide helix, onto which are appended leucine residue-like substituents. The other set, based on an inside-out approach, has a naphthalene core that mimics the two most deeply buried leucines, with substituents extending outward to mimic other features of the coactivator helical peptide. A fluorescence anisotropy-based coactivator competition assay was developed to measure the specific binding of these CBIs to the groove site on the ER-agonist complex with which coactivators interact; control ligand-binding assays assured that their interaction was not with the ligand binding pocket. The most effective CBIs were those from the pyrimidine family, the best binding with Ki values of ca. 30 .mu.M. The trithiane- and cyclohexane-based CBIs appear to be poor structural mimics, because of equatorial vs. axial conformational constraints, and the triazene-based CBIs are also conformationally constrained by amine-substituent-to-ring resonance overlap, which is not the case with the higher affinity alkyl-substituted pyrimidines. The pyrimidine-based CBIs appear to be the first small mol. inhibitors of NR coactivator binding.
IT **656822-41-2P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and in vitro biol. evaluation of triazene-, pyrimidine-, trithiane-, cyclohexane-, and naphthalene-based small mol. inhibitors of estrogen receptor .alpha. coactivator binding)
RN 656822-41-2 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, 1,3,5-trimethyl-N,N',N''-tris(2-methylpropyl)-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 3 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:1006725 HCAPLUS
DOCUMENT NUMBER: 140:64687
TITLE: Cosmetic compositions containing silicones and organogelling agents
INVENTOR(S): Ferrari, Veronique; Mondet, Jean
PATENT ASSIGNEE(S): L'Oreal, Fr.
SOURCE: PCT Int. Appl., 154 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003105788	A2	20031224	WO 2003-EP6463	20030602
WO 2003105788	A3	20040401		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

FR 2840807	A1	20031219	FR 2002-7206	20020612

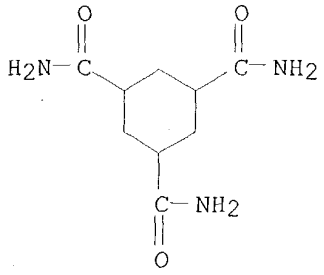
PRIORITY APPLN. INFO.: FR 2002-7206 A 20020612
US 2002-391617P P 20020627

OTHER SOURCE(S): MARPAT 140:64687

AB A cosmetic compn. comprises a liq. fatty phase contg. at least one silicone oil, structured with a gelling system. The gelling system comprises at least 1 polymer having a wt.-av. mol. wt. of 500-500,000, contg. at least 1 moiety comprising at least one polyorganosiloxane group and at least 2 groups capable of establishing hydrogen interactions, the polymer being solid at room temp. and sol. in the liq. fatty phase at 25-250.degree., and one non-polymeric organogelling agent. Thus, a lipstick contained DC-556 5, Parleam 5, hydrophobic treated pigments 10, a polyamide-silicone 15, preservative qs, N-laurylglutamic acid dibutylamide 5, and cyclopentasiloxane qs to 100%.

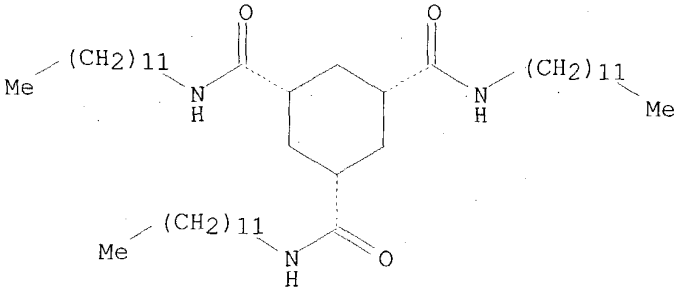
IT **99063-92-0D**, 1,3,5-Cyclohexanetricarboxamide, derivs.
189299-29-4 189299-30-7 189301-40-4
212268-42-3 212268-43-4
RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)

(cosmetic compns. contg. silicones and organogelling agents)
RN 99063-92-0 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide (6CI, 9CI) (CA INDEX NAME)



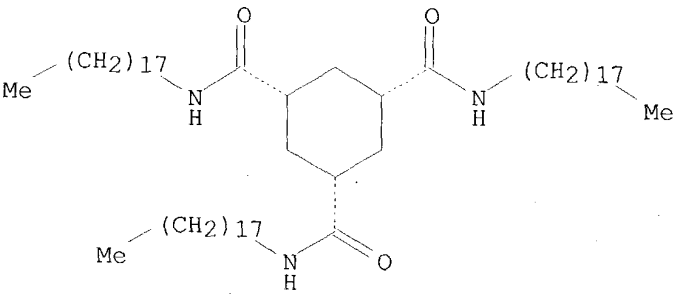
RN 189299-29-4 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tridodecyl-,
(1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 189299-30-7 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-trioctadecyl-,
(1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

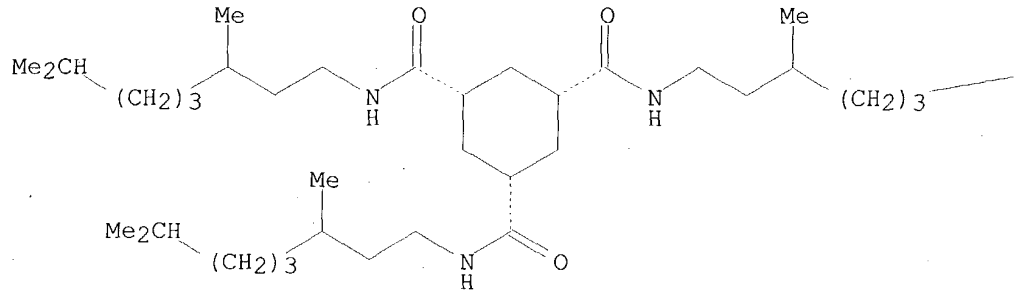
Relative stereochemistry.



RN 189301-40-4 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris(3,7-dimethyloctyl)-,
(1.alpha.,3.alpha.,5.alpha.)-[partial]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A

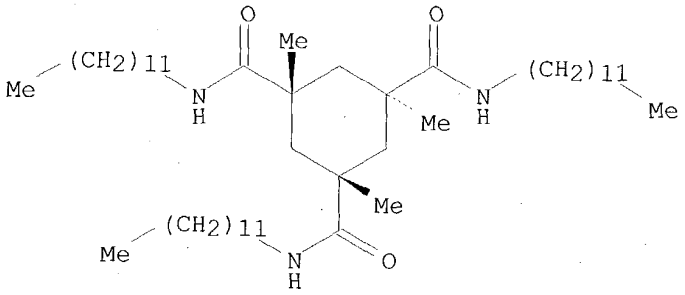


PAGE 1-B

—CHMe2

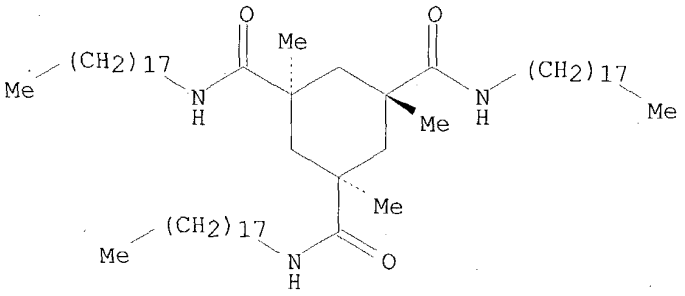
RN 212268-42-3 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tridodecyl-1,3,5-trimethyl-, (1.alpha.,3.alpha.,5.beta.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 212268-43-4 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, 1,3,5-trimethyl-N,N',N''-trioctadecyl-, (1.alpha.,3.alpha.,5.beta.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L27 ANSWER 4 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2003:990958 HCAPLUS
DOCUMENT NUMBER: 140:47044
TITLE: Cosmetic make-up or sanitary composition, structured by rigid form silicone polymers and organogelators
INVENTOR(S): Ferrari, Veronique; Mondet, Jean
PATENT ASSIGNEE(S): L'oreal, Fr.
SOURCE: Fr. Demande, 167 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2840807	A1	20031219	FR 2002-7206	20020612
WO 2003105788	A2	20031224	WO 2003-EP6463	20030602
WO 2003105788	A3	20040401		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: FR 2002-7206 A 20020612
US 2002-391617P P 20020627

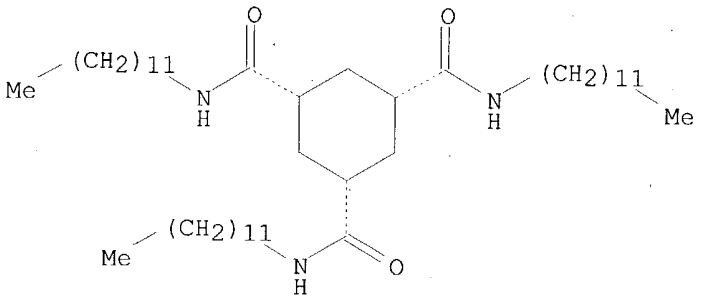
OTHER SOURCE(S): MARPAT 140:47044

AB A cosmetic make-up or sanitary compn. comprises a liq. fatty phase contg. at least a silicone oil, structured by a gelling system having at least (1) a polymer of av. mol. mass in wt. from 500 to 500 000, comprising at least a polyorganosiloxane group made up from 1 to 1000 organosiloxane units in the chain or in the form of graft, and at least two groups able to establish hydrogen interactions, the polymer being solid at the ambient temp. and sol. in the fatty liq. phase at a temp. of 25-250.degree.C, and at least (2) a not-polymeric organogelator. A lipstick contained phenyltrimethicone (DC 556, 20 cSt) 5, hydrogenated isoparaffin (Parleam) 5, hydrophobic pigments (red iron oxide, yellow titanium oxide) 10, silicone polyamide 15, preservatives q.s., organogelator (N-laurylglutamic acid dibutylamide) 5, perfume q.s., and cyclopentasiloxane D5 q.s. 100%.

IT **189299-29-4 189299-30-7 189301-40-4**
319922-90-2 319922-91-3
RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)
(cosmetic make-up or sanitary compn., structured by rigid form silicone polymers and organogelators)

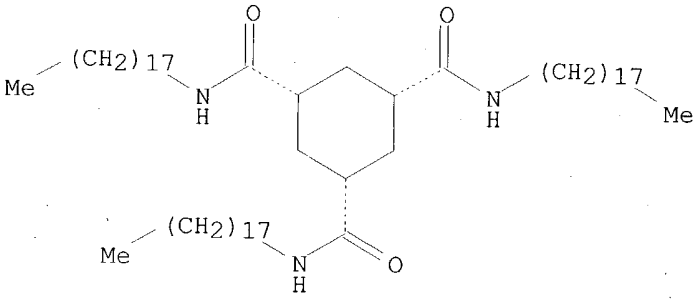
RN 189299-29-4 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tridodecyl-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 189299-30-7 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-trioctadecyl-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

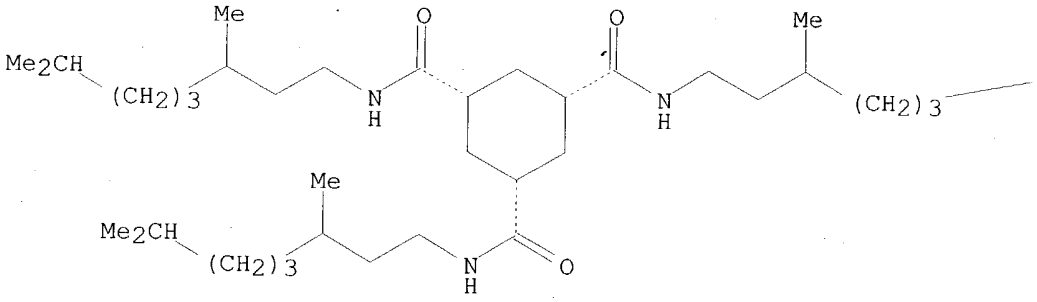
Relative stereochemistry.



RN 189301-40-4 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris(3,7-dimethyloctyl)-, (1.alpha.,3.alpha.,5.alpha.)-[partial]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



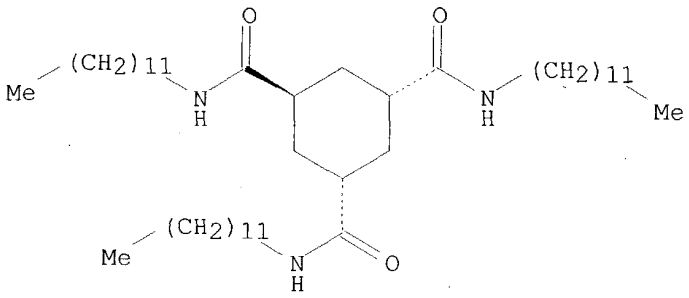
PAGE 1-B

—CHMe2

RN 319922-90-2 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tridodecyl-,

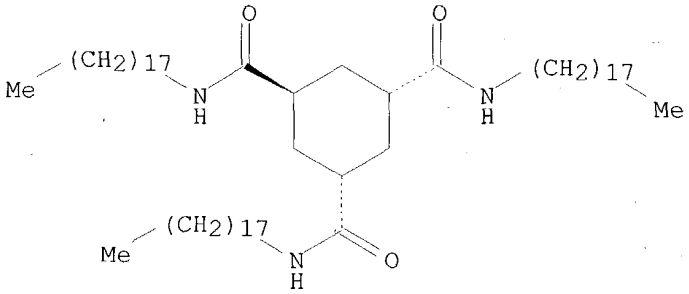
(1.alpha.,3.alpha.,5.beta.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 319922-91-3 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-trioctadecyl-,
(1.alpha.,3.alpha.,5.beta.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



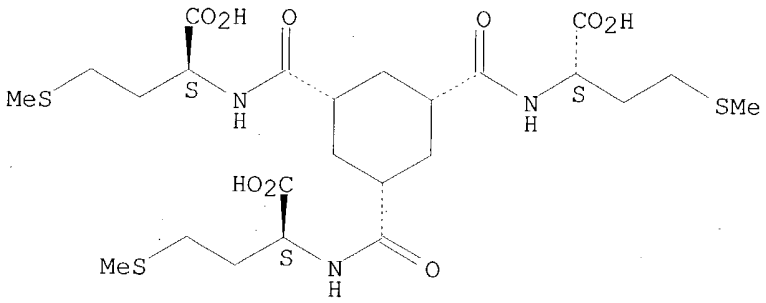
L27 ANSWER 5 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:851475 HCAPLUS
DOCUMENT NUMBER: 140:65724
TITLE: Orthogonal Self-Assembly of Low Molecular Weight Hydrogelators and Surfactants
AUTHOR(S): Heeres, Andre; Van der Pol, Cornelia; Stuart, Marc; Friggeri, Arianna; Feringa, Ben L.; Van Esch, Jan
CORPORATE SOURCE: BioMaDe Technology Foundation, Groningen, 9747, Neth.
SOURCE: Journal of the American Chemical Society (2003), 125(47), 14252-14253
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The concurrent self-assembly of new 1,3,5-trisamide-cyclohexane-based low mol. wt. hydrogelators and various surfactants in H2O gives self-assembled fibrillar networks with encapsulated micelles. This prototype system presents an example of orthogonal self-assembly, i.e., the independent formation of 2 different supramol. structures, each with their own characteristics that coexist within a single system.

IT **613243-58-6P 613243-59-7P 613243-64-4P**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(orthogonal self-assembly of low mol. wt. hydrogelators and surfactants)

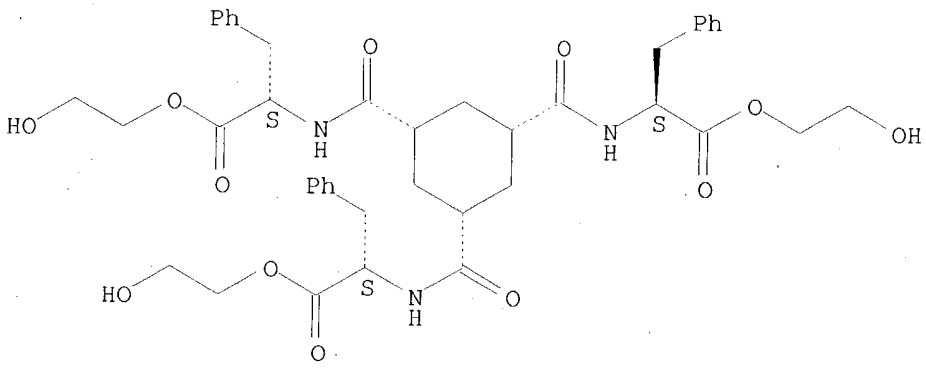
RN 613243-58-6 HCAPLUS
CN L-Methionine, N,N',N''-[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-cyclohexanetriyltricarbonyl]tris- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 613243-59-7 HCAPLUS
CN L-Phenylalanine, N,N',N''-[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-cyclohexanetriyltricarbonyl]tris-, tris(2-hydroxyethyl) ester (9CI) (CA INDEX NAME)

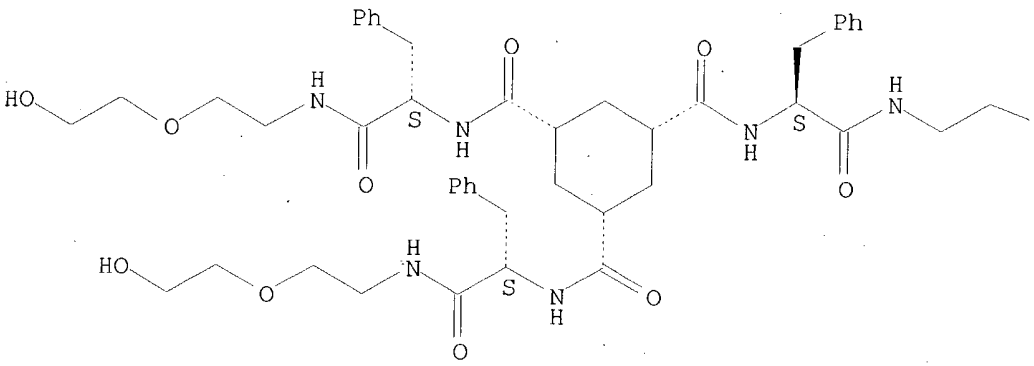
Absolute stereochemistry.



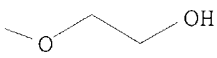
RN 613243-64-4 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris[2-[[2-(2-hydroxyethoxy)ethyl]amino]-2-oxo-1-(phenylmethyl)ethyl]-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 6 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:818262 HCAPLUS
DOCUMENT NUMBER: 139:328317
TITLE: Delivery of a substance to a pre-determined site
INVENTOR(S): Friesen, Robert Heinz Edward; Leenhouts, Cornelis Johannes; Hektor, Harm Jan; Van Esch, Johannes Henricus; Heeres, Andre; Robillard, George Thomas
PATENT ASSIGNEE(S): Applied Nanosystems B.V., Neth.
SOURCE: PCT Int. Appl., 303 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003084508	A1	20031016	WO 2003-NL256	20030404
W: AE, AG, AL, AM, AT, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EC, EE, EE, ES, FI, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1350507	A1	20031008	EP 2002-76316	20020404
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				

PRIORITY APPLN. INFO.: EP 2002-76316 A 20020404

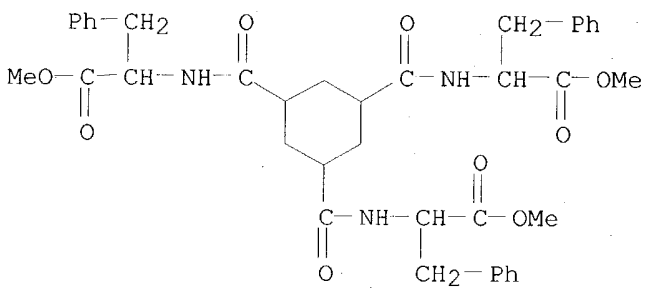
US 2002-369927P P 20020404
US 2002-370485P P 20020405
EP 2002-80481 A 20021220

OTHER SOURCE(S): MARPAT 139:328317

AB The invention is concerned with delivery vehicles for delivering a substance of interest to a predetd. site, said vehicle comprising said substance and a means for inducing availability of at least one compartment of said vehicle toward the exterior, thereby allowing access of said substance to the exterior of said vehicle at said predetd. site. The invention is further concerned with uses of said vehicle and methods for prepg. it.

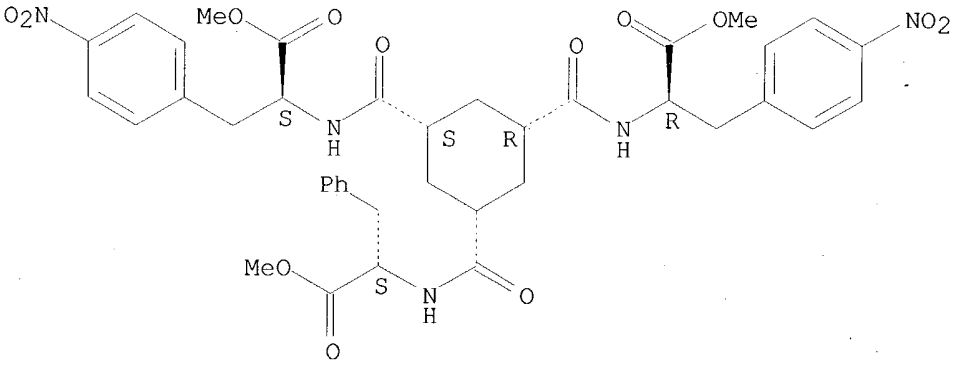
IT **613243-72-4 613243-75-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(delivery of a substance to a pre-detd. site)

RN 613243-72-4 HCAPLUS
CN Phenylalanine, N,N',N''-(1,3,5-cyclohexanetriyltricarbonyl)tris-, trimethyl ester (9CI) (CA INDEX NAME)



RN 613243-75-7 HCAPLUS
CN D-Phenylalanine, N-[[3-[[[(1S)-2-methoxy-1-[(4-nitrophenyl)methyl]-2-oxoethyl]amino]carbonyl]-5-[[[(1S)-2-methoxy-2-oxo-1-(phenylmethyl)ethyl]amino]carbonyl]cyclohexyl]carbonyl]-4-nitro-, methyl ester, stereoisomer (9CI) (CA INDEX NAME)

Absolute stereochemistry.

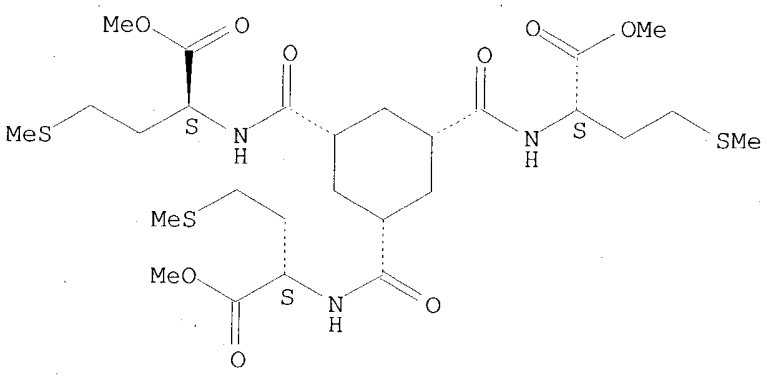


IT **613243-56-4P 613243-57-5P 613243-58-6P**
613243-59-7P 613243-60-0P 613243-61-1P
613243-62-2P 613243-63-3P 613243-64-4P
613243-68-8P 613243-69-9P 613243-71-3P
613243-73-5P 613243-74-6P 613243-76-8P
613243-78-0P 613243-79-1P 613243-81-5P
613243-82-6P 613243-87-1P 613243-94-0P
613243-95-1P 613243-96-2P 613243-99-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

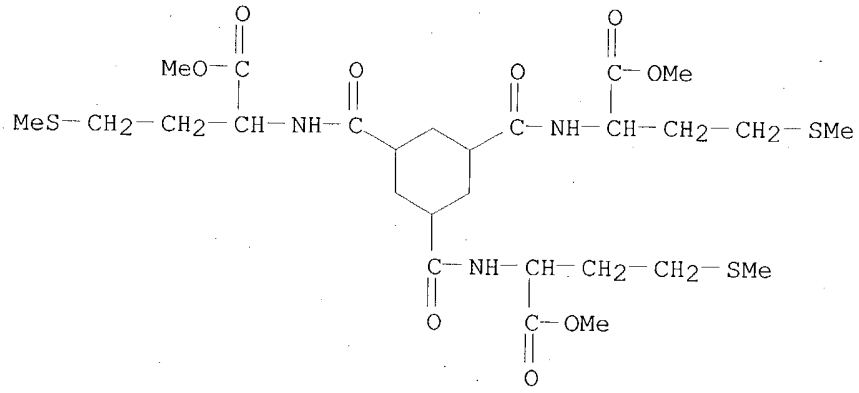
(Reactant or reagent)
(delivery of a substance to a pre-detd. site)

RN 613243-56-4 HCAPLUS
CN L-Methionine, N,N',N''-[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-cyclohexanetriyltricarbonyl]tris-, trimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

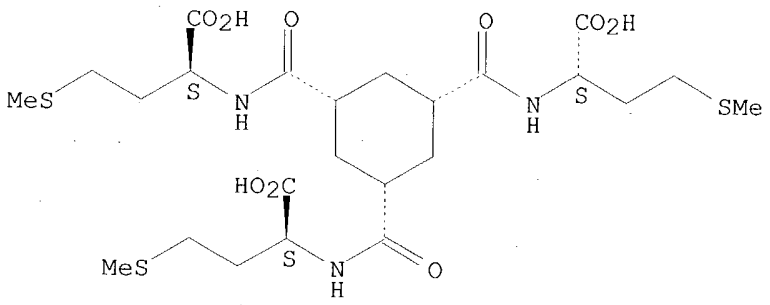


RN 613243-57-5 HCAPLUS
CN Methionine, N,N',N''-(1,3,5-cyclohexanetriyltricarbonyl)tris-, trimethyl ester (9CI) (CA INDEX NAME)



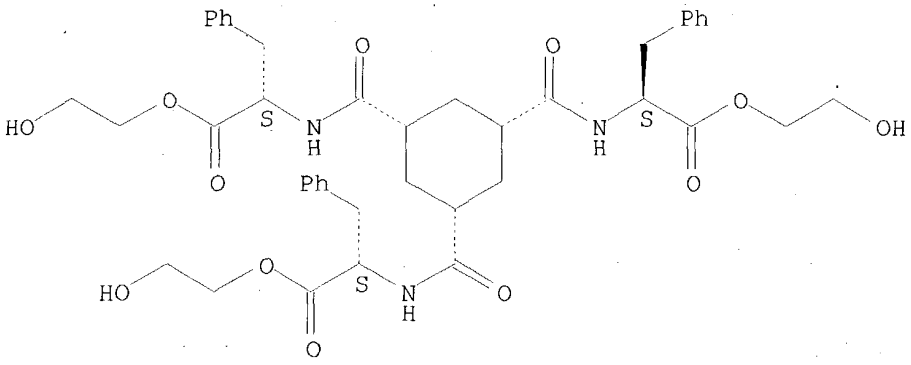
RN 613243-58-6 HCAPLUS
CN L-Methionine, N,N',N''-[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-cyclohexanetriyltricarbonyl]tris- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



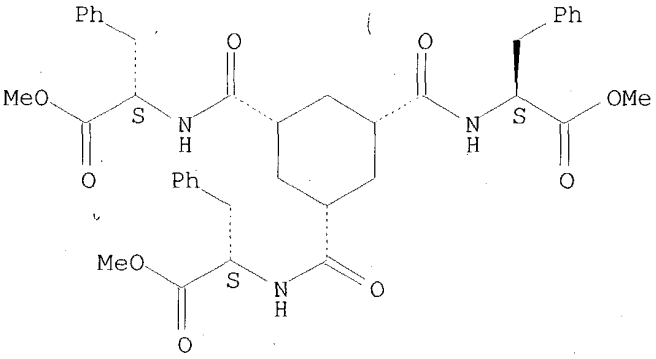
RN 613243-59-7 HCAPLUS
CN L-Phenylalanine, N,N',N''-[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-cyclohexanetriyltricarbonyl]tris-, tris(2-hydroxyethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



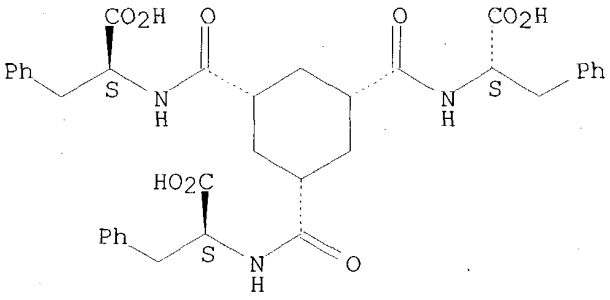
RN 613243-60-0 HCAPLUS
CN L-Phenylalanine, N,N',N''-[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-cyclohexanetriyltricarbonyl]tris-, trimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 613243-61-1 HCAPLUS
CN L-Phenylalanine, N,N',N''-[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-cyclohexanetriyltricarbonyl]tris- (9CI) (CA INDEX NAME)

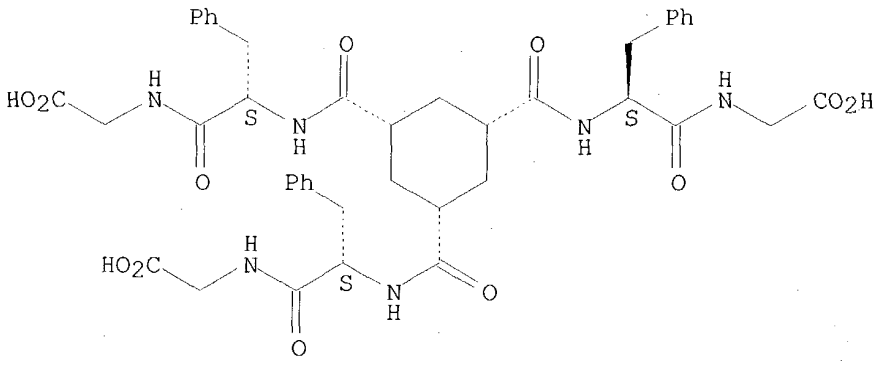
Absolute stereochemistry.



RN 613243-62-2 HCAPLUS

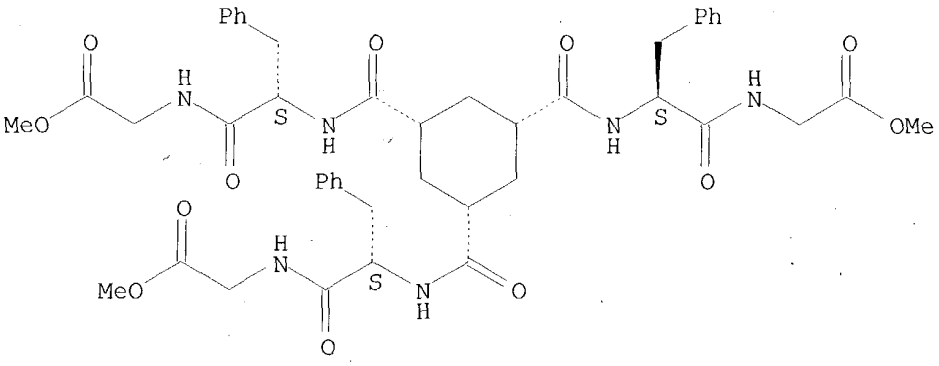
CN Glycine, 1,1',1''-[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-cyclohexanetriyltricarbonyl]tris[L-phenylalanyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 613243-63-3 HCAPLUS
CN Glycine, 1,1',1''-[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-cyclohexanetriyltricarbonyl]tris[L-phenylalanyl-, trimethyl ester (9CI) (CA INDEX NAME)

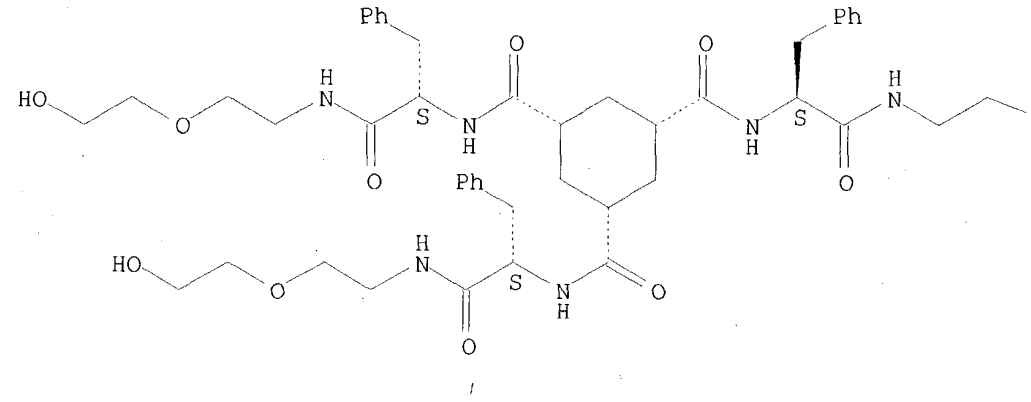
Absolute stereochemistry.



RN 613243-64-4 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris[2-[[2-(2-hydroxyethoxy)ethyl]amino]-2-oxo-1-(phenylmethyl)ethyl]-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

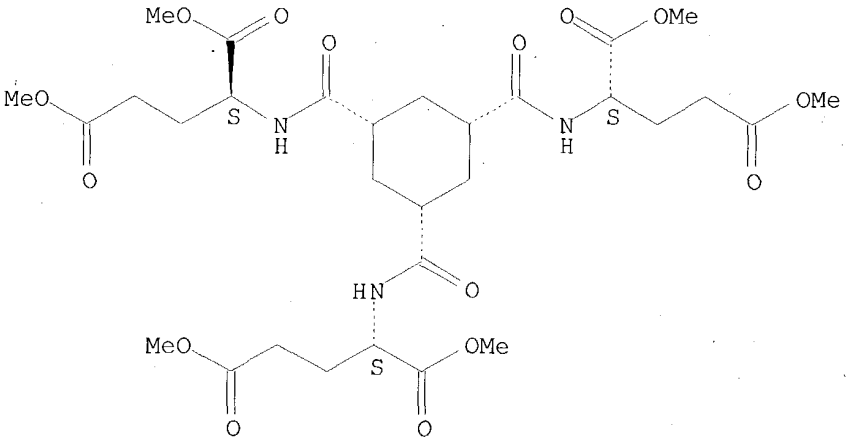
PAGE 1-A



PAGE 1-B

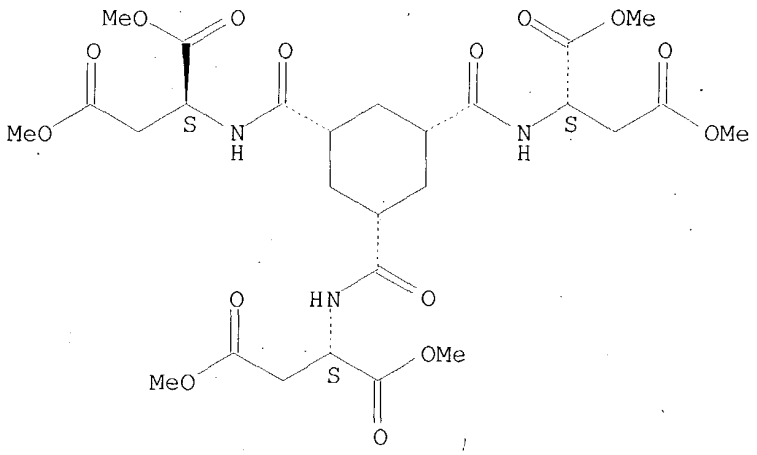
RN 613243-68-8 HCAPLUS
CN L-Glutamic acid, N,N',N''-[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-cyclohexanetriyltricarbonyl]tris-, hexamethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

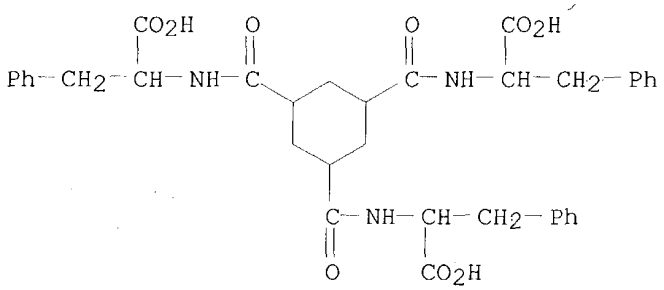


RN 613243-69-9 HCAPLUS
CN L-Aspartic acid, N,N',N''-[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-cyclohexanetriyltricarbonyl]tris-, hexamethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

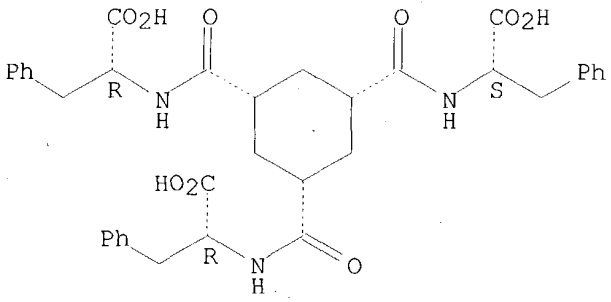


RN 613243-71-3 HCAPLUS
CN Phenylalanine, N,N',N''-(1,3,5-cyclohexanetriyltricarbonyl)tris- (9CI) (CA INDEX NAME)



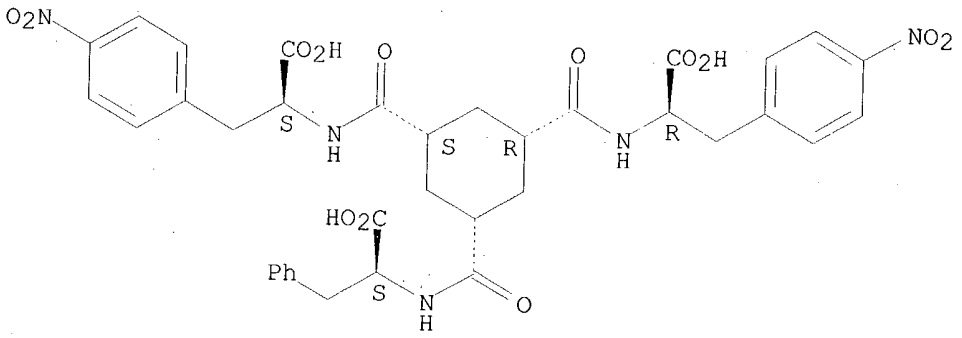
RN 613243-73-5 HCAPLUS
CN D-Phenylalanine, N,N'-[[(1.alpha.,3.alpha.,5.alpha.)-5-[[[(1S)-1-carboxy-2-phenylethyl]amino]carbonyl]-1,3-cyclohexanediyl]dicarbonyl]bis- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



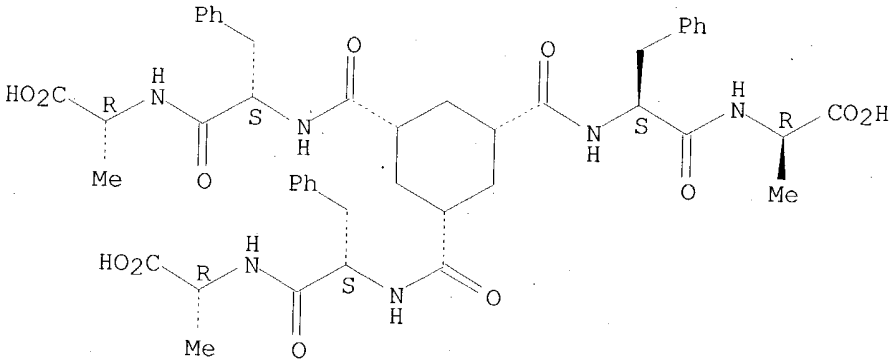
RN 613243-74-6 HCAPLUS
CN D-Phenylalanine, N-[[3-[[[(1S)-1-carboxy-2-(4-nitrophenyl)ethyl]amino]carbonyl]-5-[[[(1S)-1-carboxy-2-phenylethyl]amino]carbonyl]cyclohexyl]carbonyl]-4-nitro-, stereoisomer (9CI) (CA INDEX NAME)

Absolute stereochemistry.



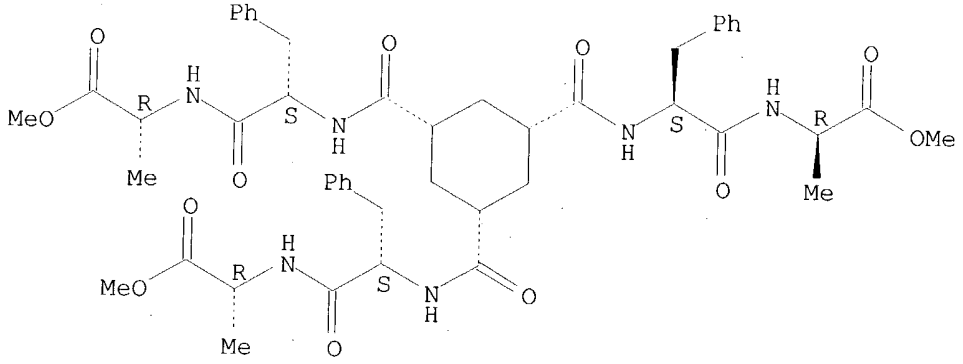
RN 613243-76-8 HCAPLUS
CN D-Alanine, 1,1',1''-[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-cyclohexanetriyltricarbonyl]tris[L-phenylalanyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



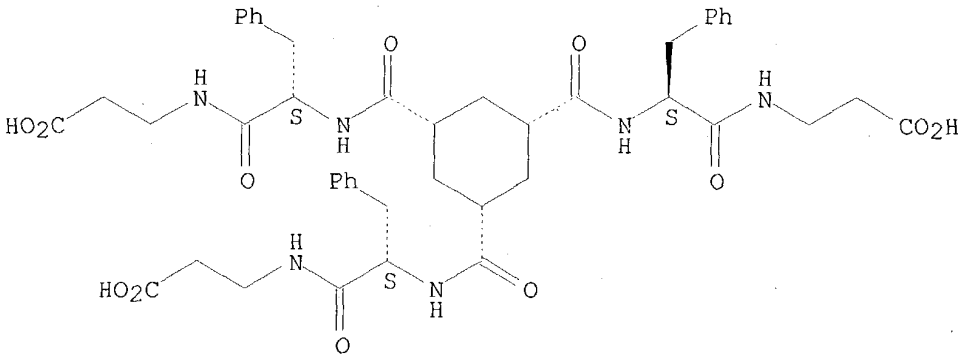
RN 613243-78-0 HCAPLUS
CN D-Alanine, 1,1',1''-[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-cyclohexanetriyltricarbonyl]tris[L-phenylalanyl-, trimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 613243-79-1 HCAPLUS
CN .beta.-Alanine, 1,1',1''-[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-cyclohexanetriyltricarbonyl]tris[L-phenylalanyl- (9CI) (CA INDEX NAME)

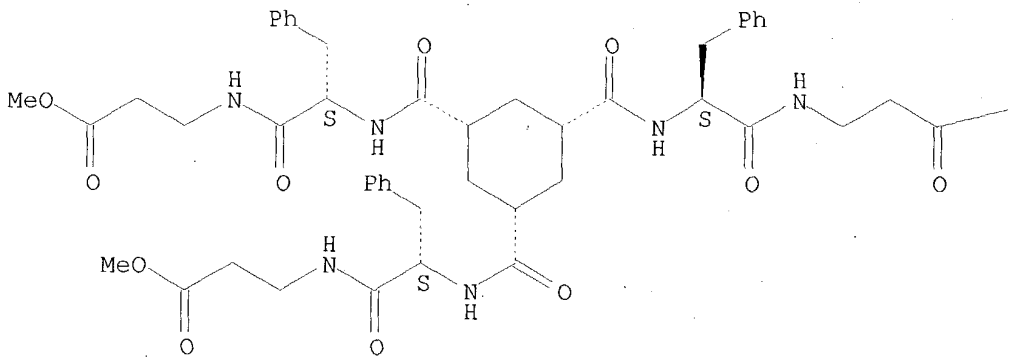
Absolute stereochemistry.



RN 613243-81-5 HCAPLUS
CN .beta.-Alanine, 1,1',1''-[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-cyclohexanetriyltricarbonyl]tris[L-phenylalanyl-, trimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



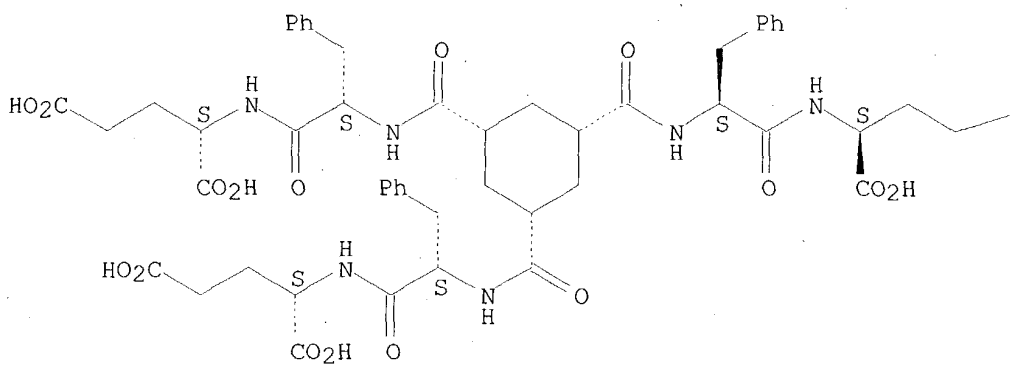
PAGE 1-B

—OMe

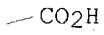
RN 613243-82-6 HCAPLUS
CN L-Glutamic acid, 1,1',1''-[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-cyclohexanetriyltricarbonyl]tris[L-phenylalanyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



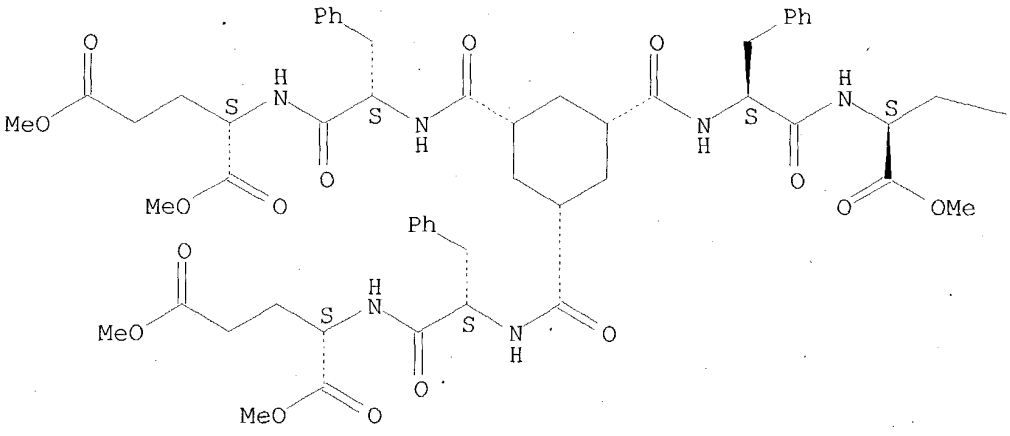
PAGE 1-B



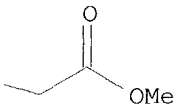
RN 613243-87-1 HCAPLUS
CN L-Glutamic acid, 1,1',1''-[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-cyclohexanetriyltricarbonyl]tris[L-phenylalanyl-, hexamethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



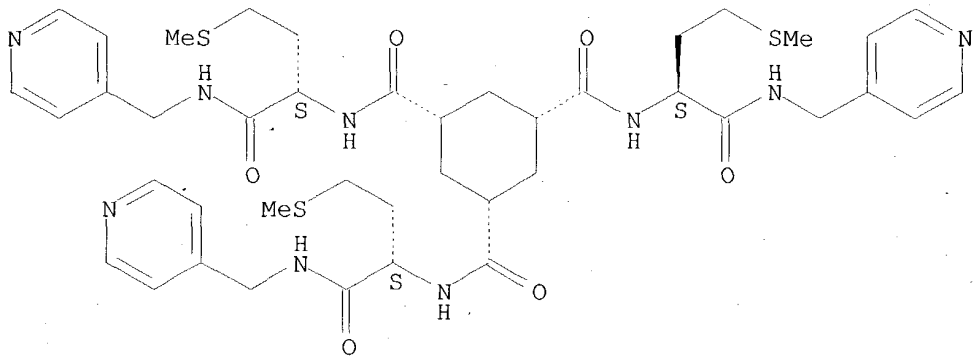
PAGE 1-B



RN 613243-94-0 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris[3-(methylthio)-1-[[(4-pyridinylmethyl)amino]carbonyl]propyl]-, (1.alpha.,3.alpha.,5.alpha.)-(9CI) (CA INDEX NAME)

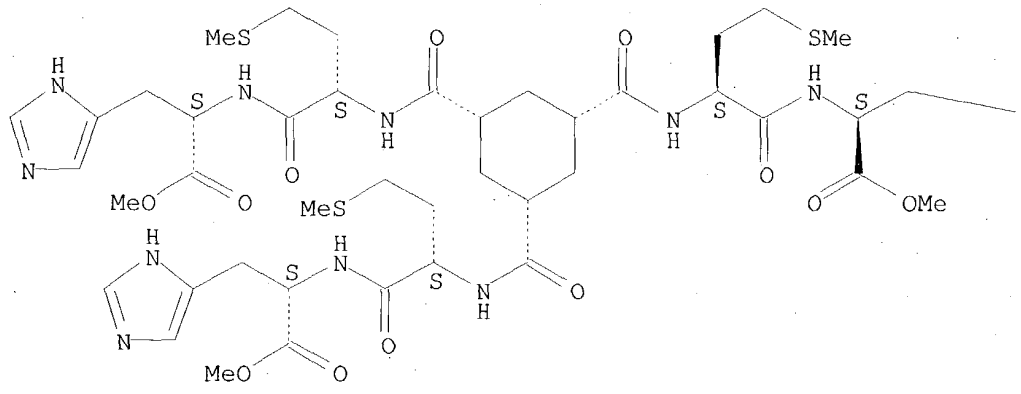
Absolute stereochemistry.



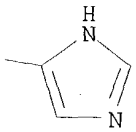
RN 613243-95-1 HCAPLUS
CN L-Histidine, 1,1',1''-[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-cyclohexanetriyltricarbonyl]tris[L-methionyl-, trimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

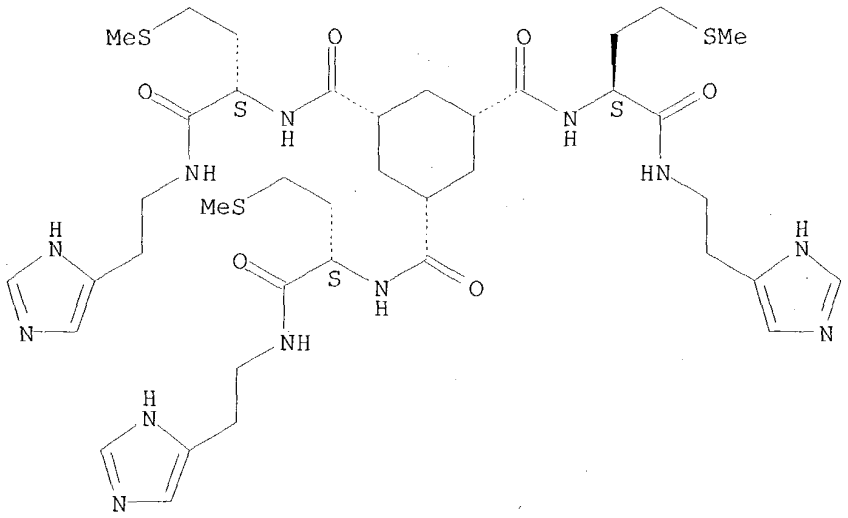


PAGE 1-B



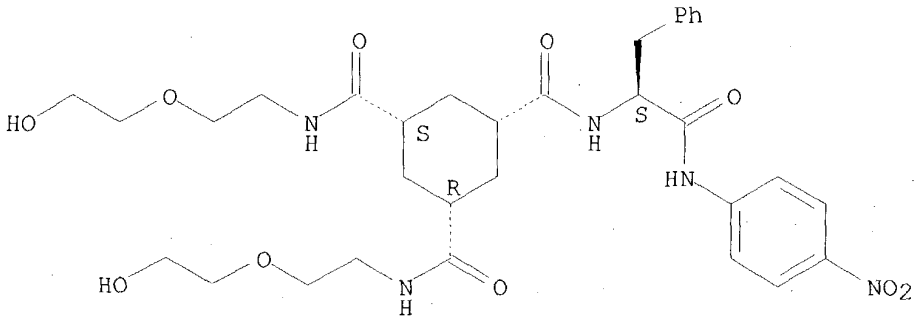
RN 613243-96-2 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris[(1S)-1-[[[2-(1H-imidazol-4-yl)ethyl]amino]carbonyl]-3-(methylthio)propyl]-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 613243-99-5 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N'-bis[2-(2-hydroxyethoxy)ethyl]-N''-[2-[(4-nitrophenyl)amino]-2-oxo-1-(phenylmethyl)ethyl]-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

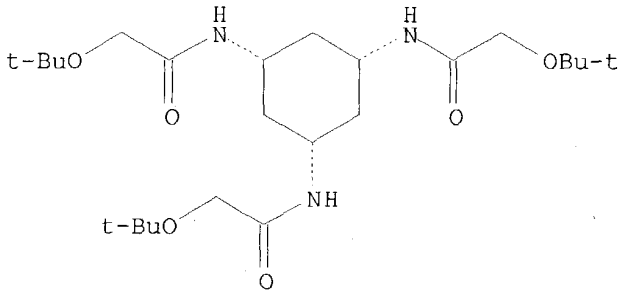
L27 ANSWER 7 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:686370 HCAPLUS
DOCUMENT NUMBER: 140:174771
TITLE: Evaluation of copper chelation agents as anti-angiogenic therapy
AUTHOR(S): Camphausen, Kevin; Sproull, Mary; Tantama, Steve; Sankineni, Sandeep; Scott, Tamalee; Menard, Cynthia; Coleman, C. Norman; Brechbiel, Martin W.
CORPORATE SOURCE: Building 10, National Cancer Institute, Radiation Oncology Branch, National Institutes of Health, Bethesda, MD, 20892-1002, USA
SOURCE: Bioorganic & Medicinal Chemistry (2003), 11(19), 4287-4293
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The design, synthesis and evaluation of N,N',N''-tris(2-pyridylmethyl)-cis,cis-1,3,5,-triaminocyclohexane (tachpyr, 1) derivs. as novel anti-angiogenic agents were performed in an in vitro endothelial cell proliferation assay to assess their cytotoxicity and selectivity. The selective nature of the anti-angiogenic agents for human umbilical vein endothelial cells (Huvec) was compared to a normal fibroblast cell line and a human Glioma cell line to evaluate these compds. N,N',N''-tris(2-mercaptoethyl)-cis,cis-1,3,5-triaminocyclohexane trihydrochloride was superior to tachpyr in terms of selectivity of its inhibitory activity toward the proliferation of Huvec compared to the fibroblast and human Glioma cell lines.

IT **658052-15-4P 658066-48-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(evaluation of copper chelation agents as antiangiogenic therapy)

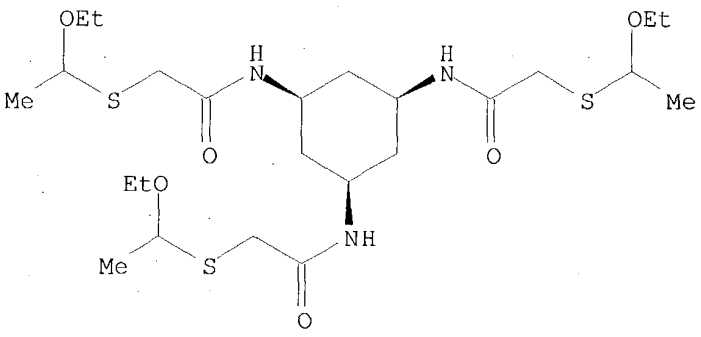
RN 658052-15-4 HCAPLUS
CN Acetamide, N,N',N''-(1.alpha.,3.alpha.,5.alpha.)-1,3,5-cyclohexanetriyltris[2-(1,1-dimethylethoxy)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 658066-48-9 HCAPLUS
CN Acetamide, N,N',N''-(1.alpha.,3.alpha.,5.alpha.)-1,3,5-cyclohexanetriyltris[2-[(1-ethoxyethyl)thio]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 8 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:561445 HCAPLUS
DOCUMENT NUMBER: 139:338257
TITLE: The chemistry of 2-alkenyl-5(4H)-oxazolones. IX. Acid-catalyzed oligomerization
AUTHOR(S): Heilmann, Steven M.; Moren, Dean M.; Krepski, Larry R.; Rasmussen, Jerald K.; Gaddam, Babu N.; Roscoe,

Stephen B.; Lewandowski, Kevin M.; McIntosh, Lester H.; Roberts, Ralph R.; Fansler, Duane D.; Szekely, Gabriella G.; Weil, David A.; Thakur, Khalid A.; Pathre, Sadanand V.; Battiste, John L.; Hanggi, Douglas A.

CORPORATE SOURCE: Organic Materials Technology Center, 3M, St. Paul, MN, USA

SOURCE: Journal of Macromolecular Science, Pure and Applied Chemistry (2003), A40(8), 755-790
CODEN: JSPCE6; ISSN: 1060-1325

PUBLISHER: Marcel Dekker, Inc.

DOCUMENT TYPE: Journal

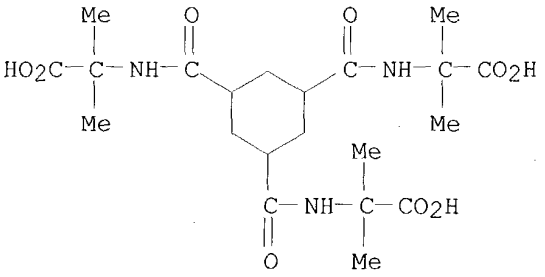
LANGUAGE: English

AB Results of the acid catalyzed oligomerization of 2-alkenyl-5(4H)-oxazolones are reported. Employing LC-MS and preparative LC methods, the oligomeric mixts. were characterized by NMR analyses and were discovered to consist of exclusively cyclic trimers to decamers, with tetramers and pentamers predominating. A nucleophilic oligomerization mechanism involving Michael addn. and C-alkylation of a ketene-aminal to protonated monomer was proposed that resulted in irreversible cyclization at the trimer propagation stage. Subsequent oligomerization proceeded via enolization of .alpha.-hydrogens on 2-substituted 5(4H)-oxazolone products and continued Michael addn. to protonated monomer. In the sense that when both enolizable hydrogens and protonated monomer are present, the oligomerization can be regarded as being "living.".

IT **616237-55-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(model compd.; prepn. of model compd. for acid-catalyzed oligomerization of 2-alkenyl-5(4H)-oxazolones)

RN 616237-55-9 HCAPLUS

CN Alanine, N,N',N''-(1,3,5-cyclohexanetriyltricarbonyl)tris[2-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 9 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2003:292147 HCAPLUS

DOCUMENT NUMBER: 139:52684

TITLE: Steric-factor-directed alternating supramolecular copolymer composed of hydrogen-bonded cyclohexanetricarboxamide units

AUTHOR(S): Takasawa, Ryoichi; Murota, Kazutoshi; Yoshikawa, Isao; Araki, Koji

CORPORATE SOURCE: Institute of Industrial Science, University of Tokyo, Tokyo, 153-8505, Japan

SOURCE: Macromolecular Rapid Communications (2003), 24(4), 335-339
CODEN: MRCOE3; ISSN: 1022-1336

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English

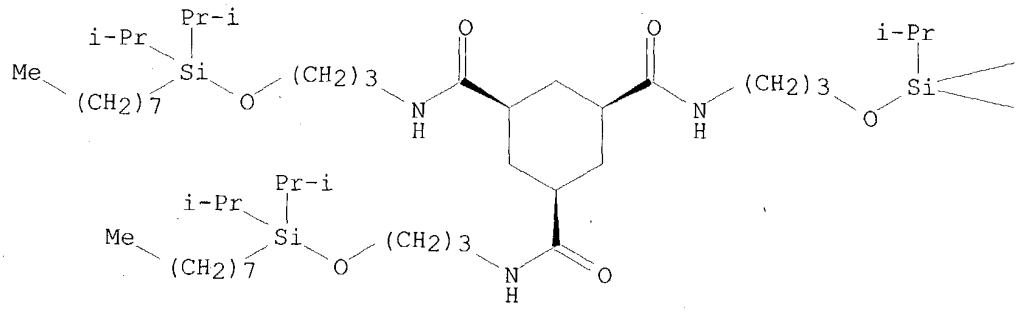
AB Hydrogen-bonded supramol. pseudo-polymers were obtained by mixing cyclohexanetricarboxamides in chloroform soln. The compds. are tris[3-(diisopropyloctylsilanyloxy)propyl]-cis,cis-1,3,5-cyclohexanetricarboxamide and tris[2-(diisopropyloctylsilanyloxy)-1-(diisopropyloctylsilanyloxymethyl)ethyl]-cis,cis-1,3,5-cyclohexanetricarboxamide. Upon evapn. of the solvent, the hydrogen-bonded supramol. assemblies formed fibrous structures. When the mixt. was up to equimolarity, the supramol. pseudo-polymer was found to have an alternating sequence, attributed to steric effects of alkylsilyl groups.

IT **489468-25-9 489468-27-1**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process)
(steric effects of substituents on alternating supramol. hydrogen-bonded cyclohexanetricarboxamide pseudopolymer structure)

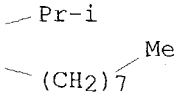
RN 489468-25-9 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris[3-[[bis(1-methylethyl)octylsilyl]oxy]propyl]-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



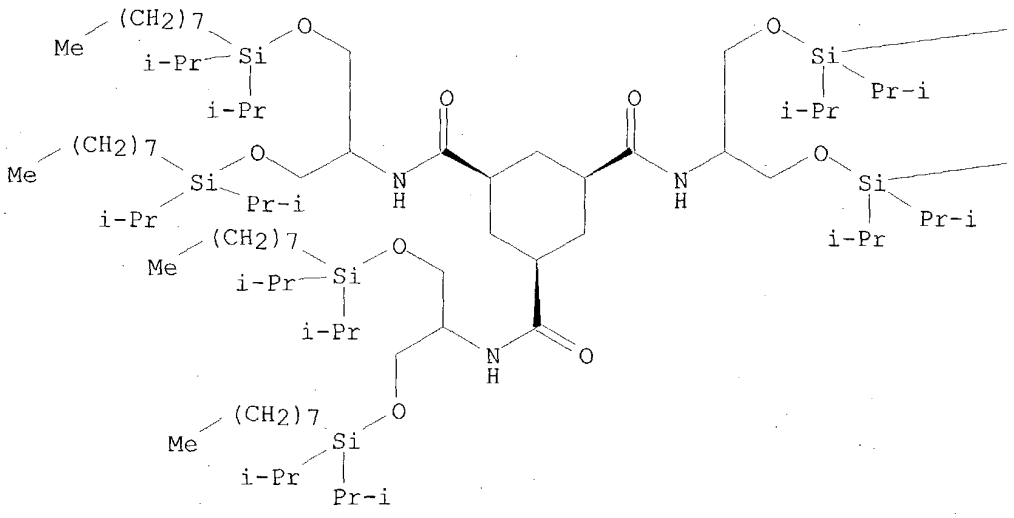
PAGE 1-B



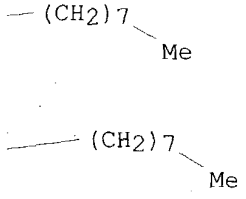
RN 489468-27-1 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris[2-[[bis(1-methylethyl)octylsilyl]oxy]-1-[[[bis(1-methylethyl)octylsilyl]oxy]methyl]ethyl]-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



PAGE 1-B



REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 10 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:944461 HCAPLUS
DOCUMENT NUMBER: 138:8260
TITLE: Use of a polar additive in a cosmetic composition containing a structured liquid oil phase by at least one organogelator to give a thixotropic character
INVENTOR(S): Livoreil, Aude; Baghdadli, Nawel
PATENT ASSIGNEE(S): L'oreal, Fr.
SOURCE: Eur. Pat. Appl., 19 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1264589	A1	20021211	EP 2002-291423	20020607
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
FR 2825618	A1	20021213	FR 2001-7474	20010607
JP 2002370926	A2	20021224	JP 2002-167454	20020607
US 2003091520	A1	20030515	US 2002-163509	20020607

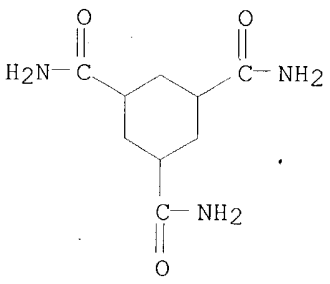
PRIORITY APPLN. INFO.: FR 2001-7474 A 20010607

AB A polar additive having a polarity parameter .delta.a .gtoreq. 7.0 (j/cm3)1/2 is used in a cosmetic compn. contg. a liq. oil phase contg. an apolar or weakly polar oil having a polarity parameter .delta.a .ltoreq. 7.0 (j/cm3)1/2 structured by at least one organogelator to give a thixotropic character. Formulation of a cosmetic compn. contg. octyldodecanol and 2-ethylhexyl palmitate is disclosed.

IT **99063-92-0,** 1,3,5-Cyclohexanetricarboxamide
RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)
(use of polar additive in cosmetic compn. contg. structured liq. oil phase by at least one organogelator to give thixotropic character)

RN 99063-92-0 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide (6CI, 9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 11 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:858259 HCAPLUS

DOCUMENT NUMBER: 138:122405

TITLE: Design, fabrication and properties of triamidecyclohexane supramolecular fibers consisted of hydrogen-bonded pseudo-polymer chains

AUTHOR(S): Takasawa, Ryoichi; Yoshikawa, Isao; Araki, Koji

CORPORATE SOURCE: Inst. of Industrial Science, Univ. of Tokyo, Tokyo, 153-8505, Japan

SOURCE: Kobunshi Ronbunshu (2002), 59(10), 616-622
CODEN: KBRBA3; ISSN: 0386-2186

PUBLISHER: Kobunshi Gakkai

DOCUMENT TYPE: Journal

LANGUAGE: Japanese

AB Triamidecyclohexane derivs. were reported to form rigid pseudo-polymer chains by triple intermol. hydrogen bonds between their amide groups. The compd. 2, tris[3-(diisopropyloctylsilyloxy)propyl]-cis,cis-1,3,5-cyclohexanetricarbox-amide, which was designed to cover its hydrogen-bonded pseudo-polymer chain by nonpolar flexible diisopropyloctylsilyl groups, was synthesized and fabricated into a sufficiently flexible supramol. fiber by spinning at 150.degree. (spinning rate was 8-11 m min-1). The IR spectra of the fiber confirmed formation of the pseudo-polymer chain by the triple intermol. hydrogen bonds between the amide groups, and the X-ray diffraction pattern showed high orientation of the pseudo-polymer chains along the fiber axis (orientation function fc = 0.6). Tensile strength of the fiber was around 1 MPa. Polarized microscopic observation indicated that the fiber did not have a uniformly oriented structure but was composed of domains in 10-50 mm scale, even after fabrication by spinning.

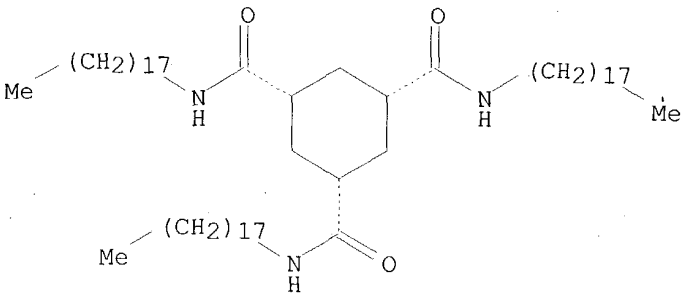
IT **189299-30-7P 489468-25-9P 489468-27-1P**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)

(fiber; design, fabrication and properties of triamidecyclohexane supramol. fibers consisted of hydrogen-bonded pseudo-polymer chains)

RN 189299-30-7 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-trioctadecyl-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

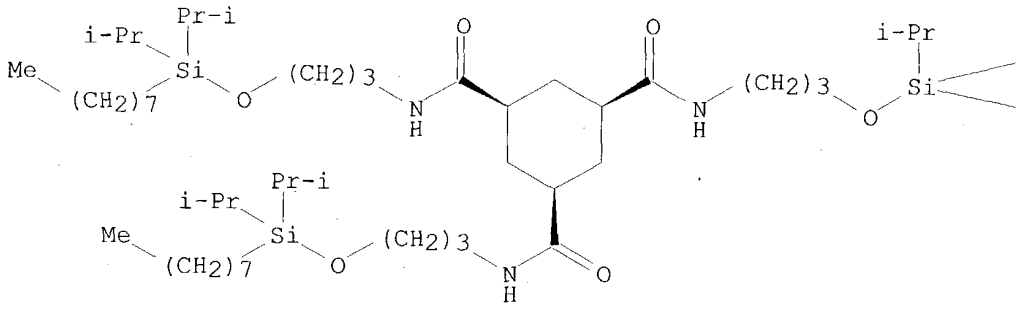


RN 489468-25-9 HCAPLUS

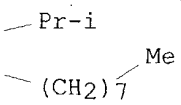
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris[3-[[bis(1-methylethyl)octylsilyl]oxy]propyl]-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



PAGE 1-B

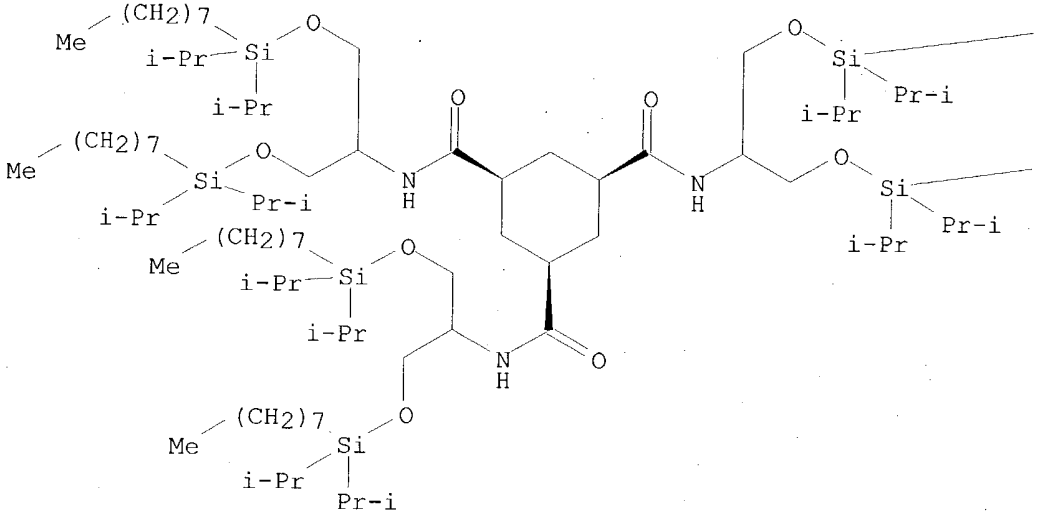


RN 489468-27-1 HCAPLUS

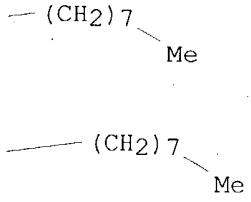
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris[2-[[bis(1-methylethyl)octylsilyl]oxy]-1-[[[bis(1-methylethyl)octylsilyl]oxy]methyl]ethyl]-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



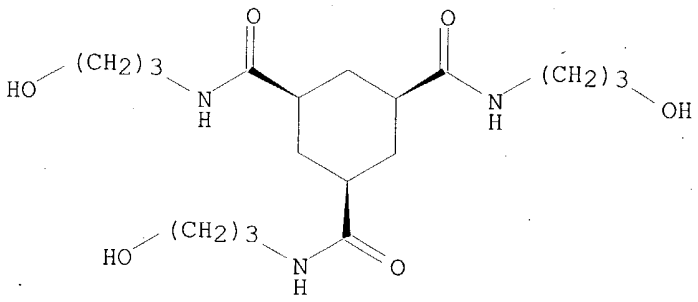
PAGE 1-B



IT **489468-24-8P 489468-26-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; design, fabrication and properties of triamidecyclohexane supramol. fibers consisted of hydrogen-bonded pseudo-polymer chains)

RN 489468-24-8 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris(3-hydroxypropyl)-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

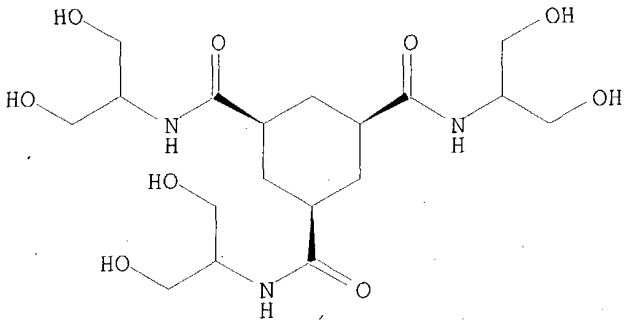
Relative stereochemistry.



RN 489468-26-0 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris[2-hydroxy-1-(hydroxymethyl)ethyl]-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L27 ANSWER 12 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:840287 HCAPLUS
DOCUMENT NUMBER: 138:182688
TITLE: Cyclotriveratrylene (CTV) as a new chiral triacid scaffold capable of inducing triple helix formation of collagen peptides containing either a native sequence or Pro-Hyp-Gly repeats
AUTHOR(S): Rump, Erik T.; Rijkers, Dirk T. S.; Hilbers, Hans W.; de Groot, Philip G.; Liskamp, Rob M. J.
CORPORATE SOURCE: Department of Haematology, University Medical Center, Utrecht, Neth.
SOURCE: Chemistry--A European Journal (2002), 8(20), 4613-4621
CODEN: CEUJED; ISSN: 0947-6539
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:182688
AB A new triacid scaffold is described based on the cone-shaped cyclotriveratrylene (CTV) mol. that facilitates the triple helical folding of peptides contg. either a unique blood platelet binding collagen sequence or collagen peptides composed of Pro-Hyp-Gly repeats. The latter were synthesized by segment condensation using Fmoc-Pro-Hyp-Gly-OH. Peptides were coupled to this CTV scaffold and also coupled to the Kemp's triacid (KTA) scaffold. After assembly of peptide H-Gly-[Pro-Hyp-Gly]2-Phe-Hyp-Gly-Glu(OAll)-Arg-Gly-Val-Glu(OAll)-Gly-[Pro-Hyp-Gly]2-NH2 (13) by an orthogonal synthesis strategy to both triacid scaffolds, followed by deprotection of the allyl groups, the mol. constructs spontaneously folded into a triple helical structure. In contrast, the non-assembled peptides did not. The melting temp. (Tm) of (+/-) CTV[CH2C-(O)N(H)Gly-[Pro-Hyp-Gly]2-Phe-Hyp-Gly-Glu-Arg-Gly-Val-Glu-Gly-[Pro-Hyp-Gly]2-NH2]3 (14) is 19.degree.C, whereas KTA[Gly-Gly-[Pro-Hyp-Gly]2-Phe-Hyp-Gly-Glu-Arg-Gly-Val-Glu-Gly-[Pro-Hyp-Gly]2-NH2]3 (15) has a Tm of 20.degree.C. Thus, it was shown for the first time that scaffolds were also effective in stabilizing the triple helix of native collagen sequences. The different stabilizing properties of the two CTV enantiomers could be measured after coupling of racemic CTV triacid to the collagen peptide, and subsequent chromatog. sepn. of the diastereomers. After assembly of the two chiral CTV scaffolds to the model peptide H-Gly-Gly-(Pro-Hyp-Gly)5-NH2 (24), the (+)-enantiomer of CTV 28b was found to serve as a better triple helix-inducing scaffold than the (-)-enantiomer 28a. In addn. to an effect of the chirality of the CTV scaffold, a certain degree of flexibility between the CTV cone and the folded peptide was also shown to

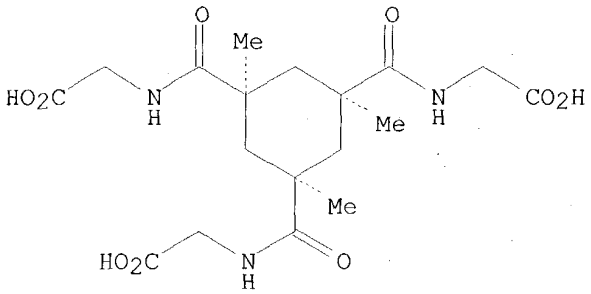
be of importance. Restricting the flexibility from two to one glycine residues resulted in a significant difference between the two collagen mimics 20a and 20b, whereas the difference was only slight when two glycine residues were present between the CTV scaffold and the peptide sequence in collagen mimics 30a and 30b.

IT **183888-51-9**
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(cyclotriveratrylene (CTV) as chiral triacid scaffold capable of inducing triple helix formation of collagen peptides contg. either a native sequence or Pro-Hyp-Gly repeats)

RN 183888-51-9 HCAPLUS

CN Glycine, N,N',N''-[[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-trimethyl-1,3,5-cyclohexanetriyl]tricarbonyl]tris- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

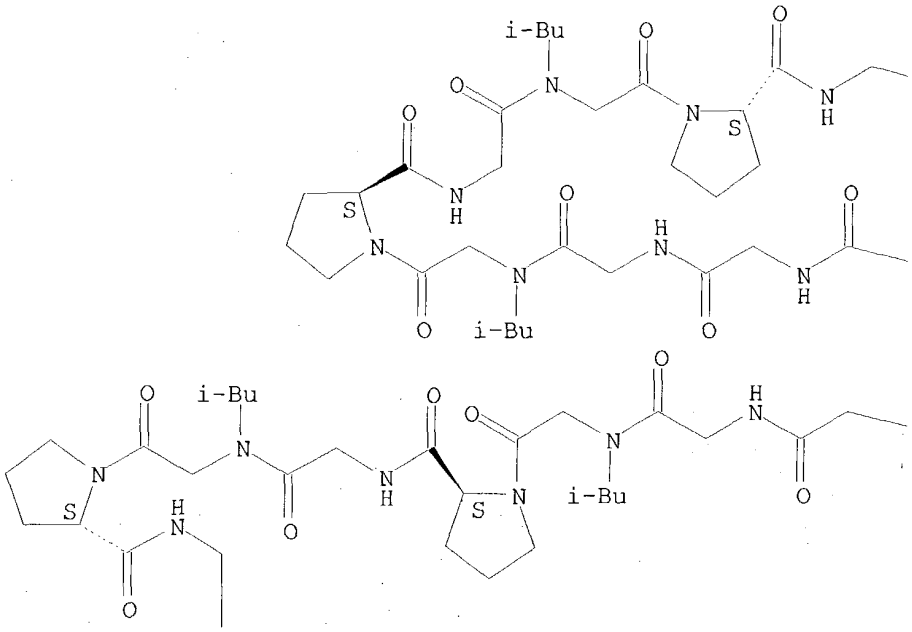
L27 ANSWER 13 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:838235 HCAPLUS
DOCUMENT NUMBER: 138:90066
TITLE: TREN (Tris(2-aminoethyl)amine): An Effective Scaffold for the Assembly of Triple Helical Collagen Mimetic Structures
AUTHOR(S): Kwak, Juliann; De Capua, Antonia; Locardi, Elsa; Goodman, Murray
CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of California, La Jolla, CA, 92093-0343, USA
SOURCE: Journal of the American Chemical Society (2002), 124(47), 14085-14091
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:90066

AB A new scaffold, TREN-(suc-OH)3 [TREN = tris(2-aminoethyl)amine, suc = succinic acid], was incorporated to assemble triple helixes composed of Gly-Nleu-Pro sequences (Nleu = N-isobutylglycine). Extensive biophys. studies, which included denaturation studies, CD and NMR spectroscopy, and mol. modeling demonstrated that TREN-[suc-(Gly-Nleu-Pro)n-NH2]3 (n = 5,6) form stable triple helical structures in soln. A comparative anal. of TREN-assembled and KTA-assembled collagen mimetics, KTA-[Gly-(Gly-Nleu-Pro)n-NH2]3 (n = 3,6; KTA = 1,3,5-trimethylcyclohexane-1,3,5-tricarboxylic acid), indicates that the flexibility of the TREN scaffold is superior to the KTA scaffold in inducing triple helicity. This effect most likely arises from the flexibility of the TREN scaffold which allows the three peptide chains to adjust their register for a tighter triple helical packing.

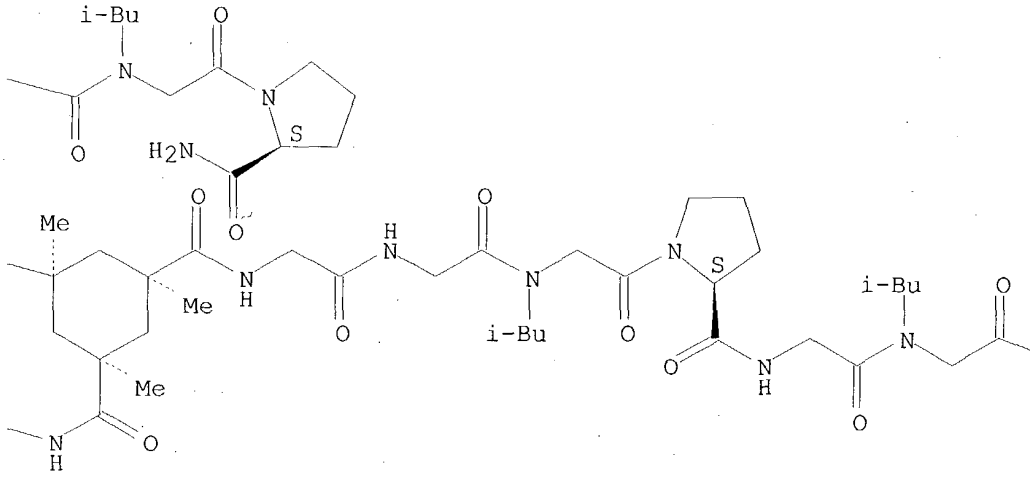
IT **191537-50-5**
RL: PRP (Properties)
(comparisons of biophys. properties of other helical peptides as collagen mimetics)
RN 191537-50-5 HCAPLUS
CN L-Prolinamide, 1,1',1''-[[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-trimethyl-1,3,5-cyclohexanetriyl]tricarbonyl]tris[glycylglycyl-N-(2-methylpropyl)glycyl-L-prolylglycyl-N-(2-methylpropyl)glycyl-L-prolylglycyl-N-(2-methylpropyl)glycyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

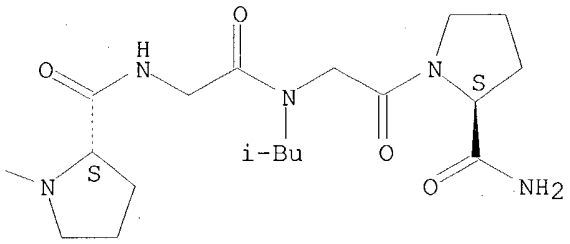
PAGE 1-A



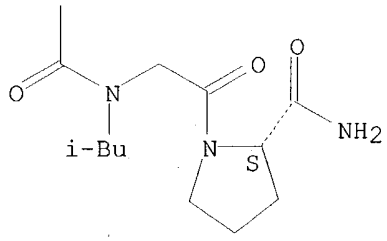
PAGE 1-B



PAGE 1-C



PAGE 2-A



REFERENCE COUNT: 60 THERE ARE 60 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 14 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:792417 HCAPLUS
DOCUMENT NUMBER: 137:318027
TITLE: Liquid crystalline compositions having high order parameter, azo dyes for the compositions, and guest-host type liquid crystal devices thereof
INVENTOR(S): Okamura, Hisashi; Kato, Takashi
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 35 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2002302674	A2	20021018	JP 2001-107254	20010405

PRIORITY APPLN. INFO.: JP 2001-107254 20010405
OTHER SOURCE(S): MARPAT 137:318027
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The liq. cryst. compns. contain compds. bearing a plurality of chromophores, .gtoreq.2 of which are linked in such a way that conjugate planes of the chromophores can align parallel to each other. The compds. may be Ia or Ia' [Da1, Da2, Da1', Da2' = substituent contg. chromophores such as those of azo dyes; Ra1-Ra6, Ra1'-Ra6' = H, substituent; 2 of Ra1-Ra6, being bonded to adjacent C, may be bonded to each other and form ring; X, Y = O, S, NR1, (substituted) C; R1 = alkyl, H]. Azo compds. shown as IIa (Ra1-Ra16 = H, substituent; 2 of Ra1-Ra16 = same as Ra1-Ra6; La1, La2 = linkage; na1, na2 = 0, 1; .gtoreq.1 of Ra7-Ra11and .gtoreq.1 of Ra12-Ra16 are azo group-contg. substituent) will be employed as Ia in the compns. Also claimed are liq. cryst. compns. contg. compds. whose .gtoreq.3 chromophores, maybe those of azo dyes or anthraquinone dyes, are linked via dendritic residues. The compds. will be represented by the formula Xb[(Lb)nb1Db]nb (Xb = dendritic residue; Db = chromophore such as those of azo dyes or anthraquinone dyes; Lb = linkage; nb1 = 0, 1; nb = 3-256 integer). Also claimed are liq. cryst. compns. contg. compds. whose .gtoreq.3 chromophores, maybe those of azo dyes or anthraquinone dyes, are linked via cyclic groups contg. .gtoreq.3 atoms bonded to chromophores directly or via linkages. The compds. will be represented by the formula Xc[(Lc)ncDc]nc1 [Xc = cyclic group capable to be bonded to (Lc)ncDc with no. of nc1; Dc = chromophore such as those of azo dyes or anthraquinone dyes; nc = 0, 1; nc1 = 3-256 integer].

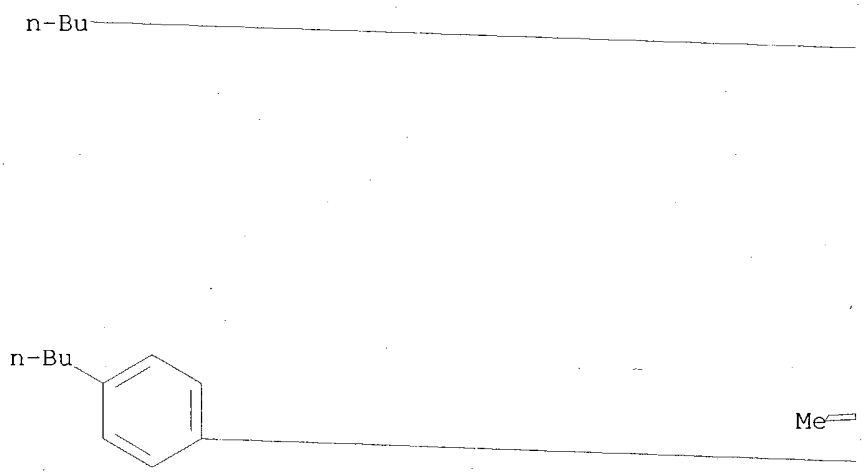
IT **472985-56-1P**
RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(dichroic liq. cryst. compns. having high order parameter, azo dyes for compns., and guest-host type LCD thereof)

RN 472985-56-1 HCAPLUS

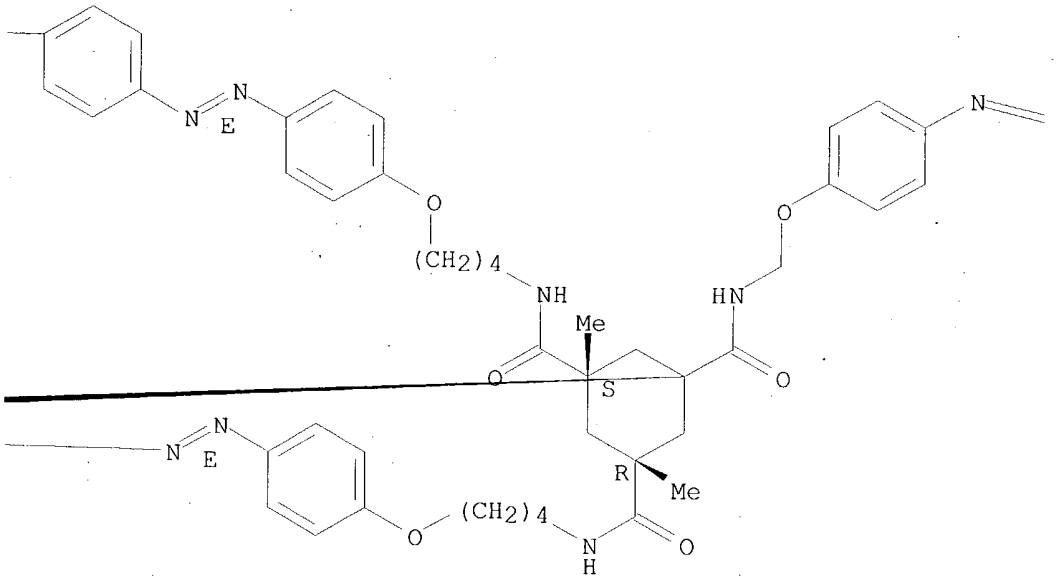
CN 1,3,5-Cyclohexanetricarboxamide, N,N'-bis[4-[4-[(1E)-(4-butylphenyl)azo]phenoxy]butyl]-N''-[[4-[(1E)-(4-butylphenyl)azo]phenoxy]methyl]-1,3,5-trimethyl-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.

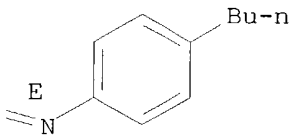
PAGE 1-A



PAGE 1-B



PAGE 1-C



L27 ANSWER 15 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:465762 HCAPLUS
DOCUMENT NUMBER: 137:52019
TITLE: Cosmetic compositions structured with a polymer containing a heteroatom and an organogelator
INVENTOR(S): Ferrari, Veronique
PATENT ASSIGNEE(S): L'oreal, Fr.
SOURCE: PCT Int. Appl., 97 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002047628	A1	20020620	WO 2000-IB2028	20001213

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,

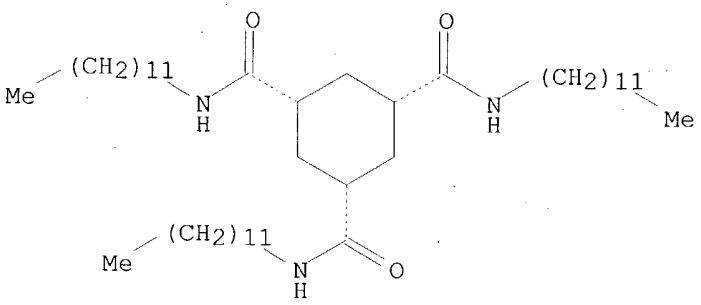
BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
AU 2001025392 A5 20020624 AU 2001-25392 20001213
WO 2002055030 A2 20020718 WO 2001-IB2780 20011212
WO 2002055030 A3 20021205
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
EP 1294342 A2 20030326 EP 2001-988098 20011212
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
PRIORITY APPLN. INFO.: WO 2000-IB2028 A 20001213
WO 2001-IB2780 W 20011212
OTHER SOURCE(S): MARPAT 137:52019

AB A physiol. acceptable compn., in particular a cosmetic compn., comprising at least one liq. fatty phase which comprises (i) at least one structuring polymer having a polymer skeleton which comprises at least one hydrocarbon-based repeating unit contg. at least one hetero atom; and (ii) at least one organogelator. A polymer skeleton is chosen from polyurethane, polyurea, and polyurethane-polyurea skeletons, and at least one structuring polymer is chosen from polyamide polymers. For example, a lipstick was prepd. contg.: Phase A - Uniclear 100 18%, GP-1 5%. isononyl isononanoate 3.33%, diisostearyl malate 15.33%, and hydrogenated polybutene 2.34%; Phase B - hydrophobic silica 3%, hydrogenated polybutene 25%, and isononyl isononanoate 12%; Phase C - pigments 7% and hydrogenated polybutene 9%. The sticks of lipstick obtained had a diam. of 12.7 mm and a hardness of 204.+-.20 g measured using a "cheese wire". The sticks of lipstick did not break during measurement of the dynamic fragility carried out on 3 sticks.

IT **189299-29-4 189299-30-7 189301-40-4**
212268-42-3 212268-43-4
RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)
(anhyd. cosmetic compns. with liq. fatty phase contg. structuring polymers and organogelators)

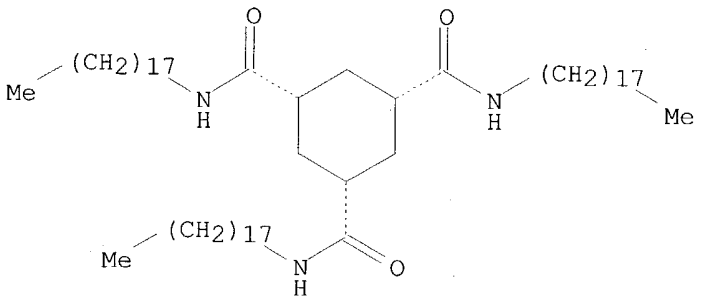
RN 189299-29-4 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tridodecyl-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 189299-30-7 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-trioctadecyl-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

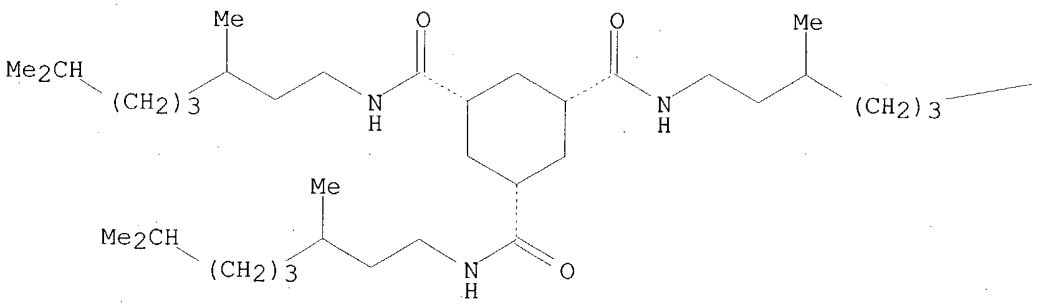
Relative stereochemistry.



RN 189301-40-4 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris(3,7-dimethyloctyl)-, (1.alpha.,3.alpha.,5.alpha.)-[partial]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A

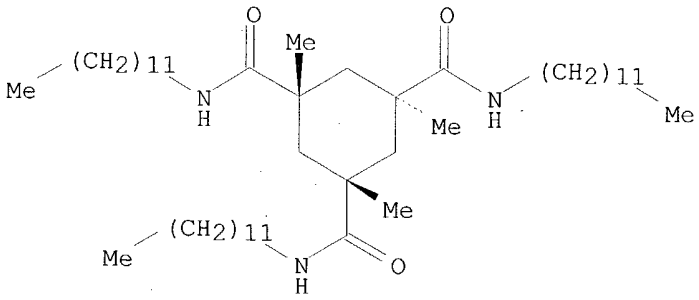


PAGE 1-B

—CHMe2

RN 212268-42-3 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tridodecyl-1,3,5-trimethyl-, (1.alpha.,3.alpha.,5.beta.)- (9CI) (CA INDEX NAME)

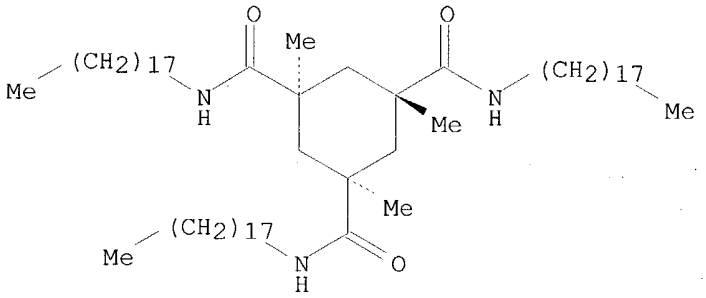
Relative stereochemistry.



RN 212268-43-4 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, 1,3,5-trimethyl-N,N',N''-trioctadecyl-,

(1.alpha.,3.alpha.,5.beta.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 16 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:403904 HCAPLUS
DOCUMENT NUMBER: 136:406922
TITLE: Dental restorative composite
INVENTOR(S): Angeletakis, Christos
PATENT ASSIGNEE(S): Kerr Corporation, USA
SOURCE: U.S., 15 pp., Cont.-in-part of U.S. 6,127,450.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 7
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6395803	B1	20020528	US 2000-567547	20000505
US 6127450	A	20001003	US 1998-93778	19980609
BR 9901799	A	20000509	BR 1999-1799	19990608
JP 2000143431	A2	20000523	JP 1999-161599	19990608
CN 1245678	A	20000301	CN 1999-108075	19990609
MX 9905338	A	20001031	MX 1999-5338	19990609
US 6384106	B1	20020507	US 2000-562190	20000502

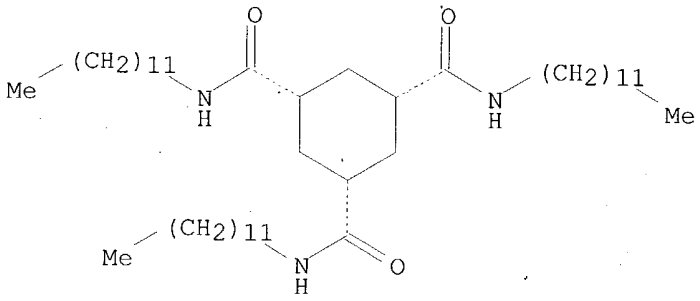
PRIORITY APPLN. INFO.: US 1998-93778 A2 19980609
OTHER SOURCE(S): MARPAT 136:406922

AB The present invention provides a resin-based dental restorative that exhibits high condensability, low volumetric shrinkage and low shrinkage stress. One or more of a rheol. modifier, dispersant and fluoro copolymer are mixed with a methacrylate resin and a fine mineral filler in amts. effective to improve the condensability of the resulting composite to achieve amalgam-like condensation, to reduce the volumetric shrinkage during polymn., to improve wear resistance, and to provide a composite with generally improved phys. properties. Thus, a resin formulation was prepd. from bis-GMA 3.0, triethylene glycol dimethacrylate 24.7, ethoxylated bisphenol A dimethacrylate 71.1, camphorquinone 0.17, 2-hydroxy-4-methoxy benzophenone 0.49, and BHT 0.05% by wt. This was mixed with a filler compn. consisting of barium aluminum silicate (silanized) 91.4, hydrophobic fumed silica (TS-530) 4.3, and fumed silica (OX-50) 4.3% by wt. The use of the rheol. modifier reduced the vol. of shrinkage significantly.

IT **189299-29-4 189299-29-4D**, alkyl derivs.
RL: MOA (Modifier or additive use); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(dental restorative composite)

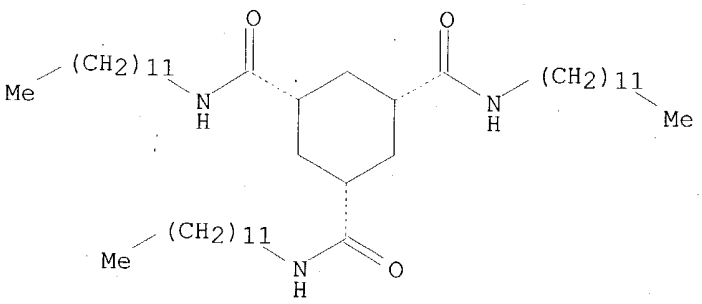
RN 189299-29-4 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tridodecyl-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 189299-29-4 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tridodecyl-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 17 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:185110 HCAPLUS
DOCUMENT NUMBER: 136:247832
TITLE: Preparation of sialic acid dendrimers as multivalent neuraminidase inhibitors and anti-influenza agents
INVENTOR(S): Wu, Wen-Yang; Dowle, Michael Dennis; Jin, Betty; Macdonald, Simon John Fawcett; Mason, Andrew McMurtrie; McConnell, Darryl; Watson, Keith
PATENT ASSIGNEE(S): Biota Scientific Management Pty. Ltd., Australia
SOURCE: PCT Int. Appl., 85 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002020514	A1	20020314	WO 2001-AU1128	20010907

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,

LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL,
PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG,
US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2001085601	A5	20020322	AU 2001-85601	20010907	
EP 1315719	A1	20030604	EP 2001-964755	20010907	
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR					
BR 2001013755	A	20030708	BR 2001-13755	20010907	
JP 2004507564	T2	20040311	JP 2002-525135	20010907	
US 2004058853	A1	20040325	US 2003-363988	20031014	
PRIORITY APPLN. INFO.:			AU 2000-10	A 20000908	
			WO 2001-AU1128	W 20010907	

OTHER SOURCE(S): MARPAT 136:247832
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention relates to a dendrimer compds. I in which : X is O or CH; R2 is azido, hydroxy, guanidino, amino, amidine, imidate; R2 is acyl or sulfonyl; Y is O, substituted amine; CG is a core group selected from an optionally substituted cyclic, straight or branched group or a combination thereof having from 1 to 200 atoms in its backbone, in which the backbone atoms are selected from C, N, O and S; and L is a linking group of from 0 to 20 backbone atoms, in which the backbone and terminal atoms are selected from C, N, O and S; or a pharmaceutically acceptable salt or deriv. thereof which comprises three or more neuraminidase-binding groups attached to a spacer or linking group, in which the neuraminidase-binding group is a compd. which binds to the active site of influenza virus neuraminidase, but is not cleaved by the neuraminidase. The invention also relates to processes for the prepn. of the multimeric compd. defined above, pharmaceutical compns. contg. them, or methods for the treatment and/or prophylaxis of a viral infection involving them. Thus, dendrimer II.3CF3CO2H salt [R1 = guanidino, R2 = acetyl, Y = O, L = CON(CH2)6] was prepd. and tested in mice as neuraminidase inhibitor and anti-influenza agent (dose = 0.01-1 mg/kg).

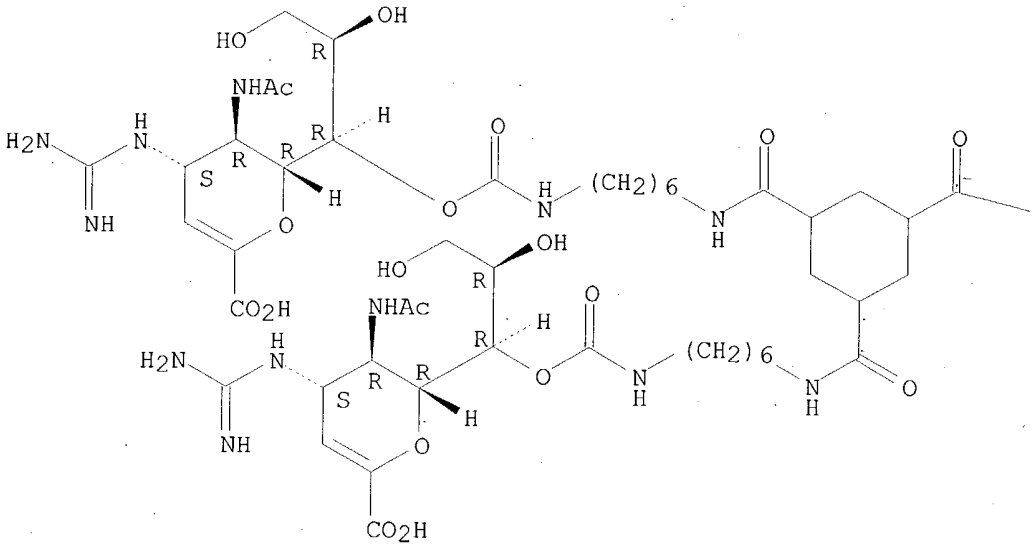
IT **403660-73-1P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of sialic acid dendrimers as multivalent neuraminidase inhibitors and antiinfluenza agents)

RN 403660-73-1 HCAPLUS

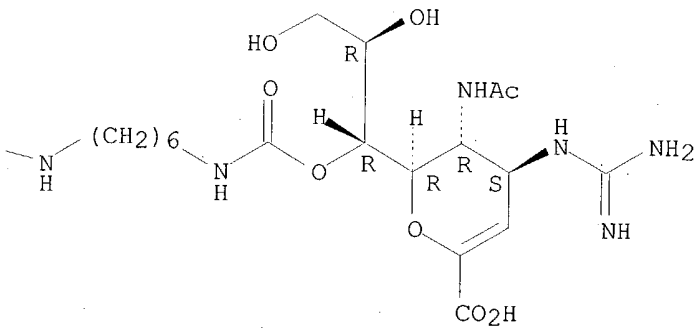
CN D-glycero-D-galacto-Non-2-enonic acid, 5-(acetylamino)-4-[(aminoiminomethyl)amino]-2,6-anhydro-3,4,5-trideoxy-, 7,7',7''-[1,3,5-cyclohexanetriyltris(carbonylimino-6,1-hexanediyl)]tris[carbamate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



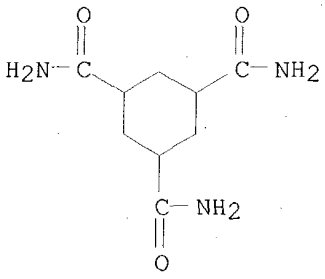
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 18 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:490016 HCAPLUS
DOCUMENT NUMBER: 135:227474
TITLE: Anionic Polymerization of an Acrylonitrile Trimer Studied by Photoelectron Spectroscopy
AUTHOR(S): Fukuda, Yuji; Ichihashi, Masahiko; Terasaki, Akira; Kondow, Tamotsu; Osoda, Kazuhiko; Narasaka, Koichi
CORPORATE SOURCE: Department of Chemistry School of Science, The University of Tokyo, Bunkyo-ku Tokyo, 113-0033, Japan
SOURCE: Journal of Physical Chemistry A (2001), 105(30), 7180-7184
CODEN: JPCAFH; ISSN: 1089-5639
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A photoelectron spectrum of an acrylonitrile (AN:CH2:CHCN) trimer anion,

(AN)3-, produced by electron impact on an acrylonitrile cluster was measured, and was compared with that of a mol. anion of 1,3,5-cyclohexanetricarbonitrile (c-HTCN) in the triequatorial form, which was first synthesized in the present expt. A comparison of the vertical detachment energies of (AN)3- and the mol. anion lead us to conclude that (AN)3- is assigned as one of the stereoisomers (diaxial form) of c-HTCN (-) on the basis of our previous studies refs. 13, 14, and 20-22 [Tsukuda, T.; Kondow, T. J. Chem. Phys. 1991, 95, 6989. Tsukuda, T.; Kondow, T. J. Am. Chem. Soc. 1994, 116, 9555. Ichihashi, M.; Tsukuda, T.; Nonose, S.; Kondow, T. J. Phys. Chem. 1995, 99, 17354. Fukuda, Y.; Tsukuda, T.; Terasaki, A.; Kondow, T. Chem. Phys. Lett. 1995, 242, 121. Fukuda, Y.; Tsukuda, T.; Terasaki, A.; Kondow, T. Chem. Phys. Lett. 1996, 260, 423.].

IT **99063-92-0P**, 1,3,5-Cyclohexanetricarboxamide
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(in prepn. and anionic polymn. of acrylonitrile trimer studied by photoelectron spectroscopy)

RN 99063-92-0 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide (6CI, 9CI) (CA INDEX NAME)



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

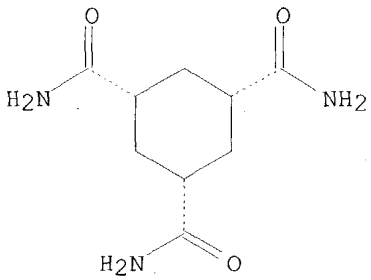
L27 ANSWER 19 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:348061 HCAPLUS
DOCUMENT NUMBER: 135:137227
TITLE: A conformational study of cyclohexane-1,3,5-tricarbonitrile derivatives
AUTHOR(S): Chuang, Tsung-Hsun; Fang, Jim-Min
CORPORATE SOURCE: Department of Chemistry, National Taiwan University, Taipei, 106, Taiwan
SOURCE: Journal of the Chinese Chemical Society (Taipei, Taiwan) (2001), 48(2), 193-200
CODEN: JCCTAC; ISSN: 0009-4536
PUBLISHER: Chinese Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:137227

AB Cyclohexane-1,3,5-tricarbonitrile reached equil. having 1,3-cis-1,5-cis and 1,3-cis-1,5-trans isomers in a ratio of 3:7. The cis,cis-isomer preferred the conformation with three equatorial cyano groups, whereas the cis,trans-isomer displayed two cyano groups in the equatorial position and another cyano group in the axial position. Condensation of cis,cis-cyclohexane-1,3,5-tricarbonitrile with L-(S)-valinol with catalysis by ZnCl2 in refluxing 1,2-dichlorobenzene afforded two isomeric cyclohexane-1,3,5-trioxazolines in favor of the 1,3-cis-1,5-trans isomer. Metalation of cis,cis-cyclohexane-1,3,5-tricarbonitrile, followed by alkylations with di-Me sulfate, benzyl bromide or allyl bromide, gave the corresponding trialkylation products with predominance of 1,3-cis-1,5-trans isomers. The cis,trans-isomer showed two cyano groups

in the axial position and another cyano group in the equatorial position, whereas the cis,cis-isomer exhibited three axial cyano groups. Treatment of tri-Me cis,cis-cyclohexane-1,3,5-tricarboxylate with lithium diisopropylamide and di-Me sulfate afforded mainly the tri-Me ester of Kemp's triacid, which showed three axial carboxylate groups. The interplay of two competitive factors, i.e., the steric effect of incoming electrophiles and the dipole-dipole interactions of the cyano or carboxylate groups, may give different stereoselectivities in these reaction systems.

IT **168280-45-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(conformational study of cyclohexane-1,3,5-tricarbonitrile derivs.)
RN 168280-45-3 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

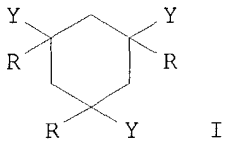


REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 20 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:45914 HCAPLUS
DOCUMENT NUMBER: 134:105647
TITLE: Solid form cosmetic compositions comprising an oil and a specific gelling agent
INVENTOR(S): Livoreil, Aude; Mougin, Nathalie
PATENT ASSIGNEE(S): L'oreal, Fr.
SOURCE: Eur. Pat. Appl., 12 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1068854	A1	20010117	EP 2000-401661	20000613
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
FR 2796276	A1	20010119	FR 1999-9178	19990715
FR 2796276	B1	20030516		
US 6372235	B1	20020416	US 2000-617131	20000714
JP 2001058915	A2	20010306	JP 2000-216708	20000717

PRIORITY APPLN. INFO.: FR 1999-9178 A 19990715
OTHER SOURCE(S): MARPAT 134:105647
GI



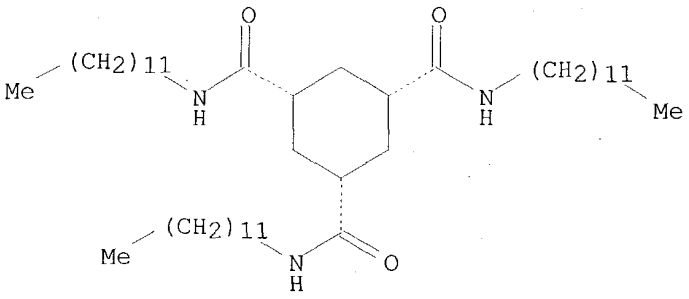
I

AB Solid form cosmetic compns. comprising an oil and gelling agent I are disclosed. The compns. are in the form of translucent anhyd. stick which are non-transferable. A compn. contg. I [R = H, Y = CONHR' (R' = C12 alkyl)] 200 mg, and isododecane 5 mL was prepd. A solid stick contained above compn. 0.8, pigments (iron oxide) 0.5 g, isododecane 16, and parleam oil 4 mL.

IT **189299-29-4 189299-30-7 189301-40-4**
319922-90-2 319922-91-3
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
(solid form cosmetic compns. comprising oil and specific gelling agent)

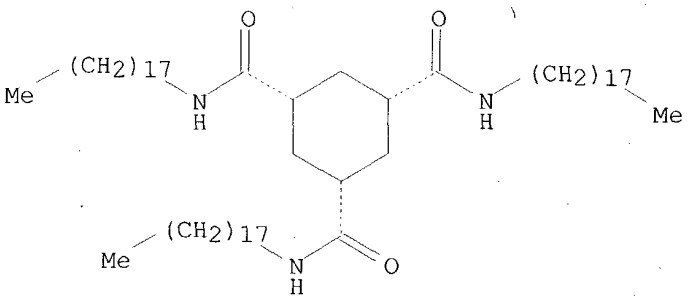
RN 189299-29-4 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tridodecyl-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 189299-30-7 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-trioctadecyl-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

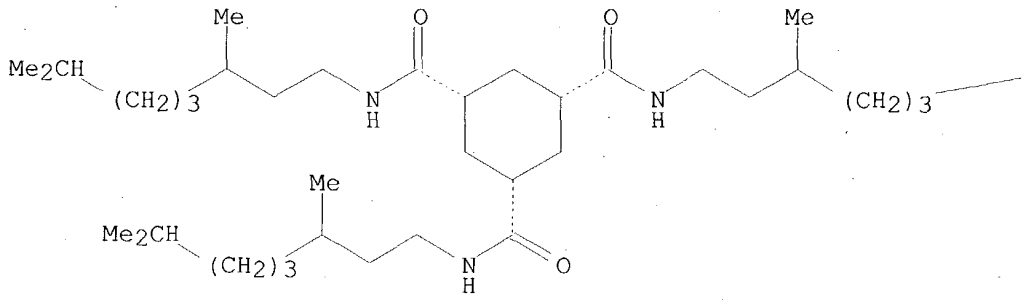
Relative stereochemistry.



RN 189301-40-4 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris(3,7-dimethyloctyl)-, (1.alpha.,3.alpha.,5.alpha.)-[partial]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A

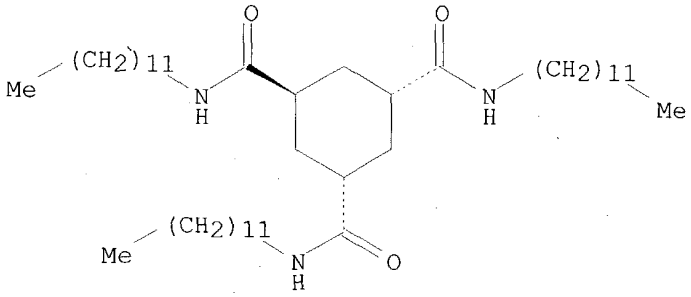


PAGE 1-B

—$CHMe_2$

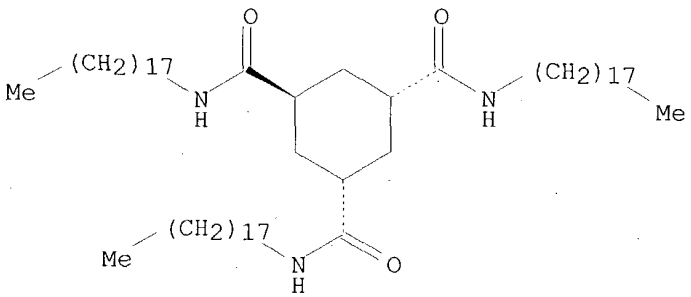
RN 319922-90-2 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tridodecyl-, (1.alpha.,3.alpha.,5.beta.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 319922-91-3 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-trioctadecyl-, (1.alpha.,3.alpha.,5.beta.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



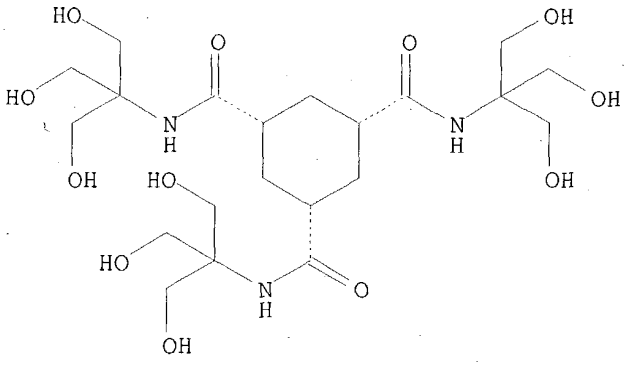
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 21 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:690425 HCAPLUS
DOCUMENT NUMBER: 134:4731
TITLE: One-step coupling of tris(hydroxymethyl)aminomethane to aliphatic and aromatic carboxylic acids
AUTHOR(S): Villanueva, Ignacio; Hernandez, Bernadette; Chang, Virginia; Heagy, Michael D.
CORPORATE SOURCE: Department of Chemistry, New Mexico Institute of Mining and Technology, Socorro, NM, 87801, USA
SOURCE: Synthesis (2000), (10), 1435-1438
CODEN: SYNTBF; ISSN: 0039-7881
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:4731

AB A convenient and general method was established to append tri-, hexa-, and nonadentate ligands about an arom. or aliph. core. This approach allows a variety of com. available carboxylates to be transformed to their N-[tris(hydroxymethyl)methyl]carboxamides in one step. The selective activation of the acid functionality to form the polyhydroxylated dendritic cores was achieved using the acyl transfer agent N-ethoxycarbonyl-2-ethoxy-1,2-dihydroquinoline (EEDQ).

IT **308357-62-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of aliph. and arom. carboxamides from tris(hydroxymethyl)aminomethane)
RN 308357-62-2 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris[2-hydroxy-1,1-bis(hydroxymethyl)ethyl]-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 22 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:421213 HCAPLUS
DOCUMENT NUMBER: 133:59703
TITLE: Association of compounds in carbon dioxide and the gels and/or microcellular foams therefrom for fracturing subterranean formations
INVENTOR(S): Beckman, Eric J.; Hamilton, Andrew D.; Huang, Zhihua; Carr, Andrew; Enick, Robert M.
PATENT ASSIGNEE(S): Yale University, USA
SOURCE: PCT Int. Appl., 101 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000035998	A2	20000622	WO 1999-US29574	19991215
WO 2000035998	A3	20001019		

W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 1998-112188P P 19981215
US 1999-166164P P 19991118

AB The viscosity of supercrit. CO2 is increased by combining a compd. having a CO2-philic functional group, such as a fluoroalkyl, siloxane or alkylene oxide group, and an aggregating functional group, such as an amide, urea, carboxylic acid, or thiourea group, which enables the compd. to form a supramol. network in soln. with supercrit. CO2. The compd. is aggregated in soln. to form a supramol. network such that the viscosity of the supercrit. CO2 with the supramol. network is greater than that of the starting supercrit. CO2. The gels are useful as fracturing fluids, solvents for paints and oils, in coatings or insulating materials, or as fillers (no data). A microcellular foam is prepd. by combining a compd. having a CO2-philic functional group and an aggregating functional group which enables the compd. to form a supramol. network in soln. with supercrit. CO2, then removing the CO2. The microcellular foams can also be used for low-d. structural parts, high-temp. insulation, sepn. media, adsorbents, and catalyst supports (no data).

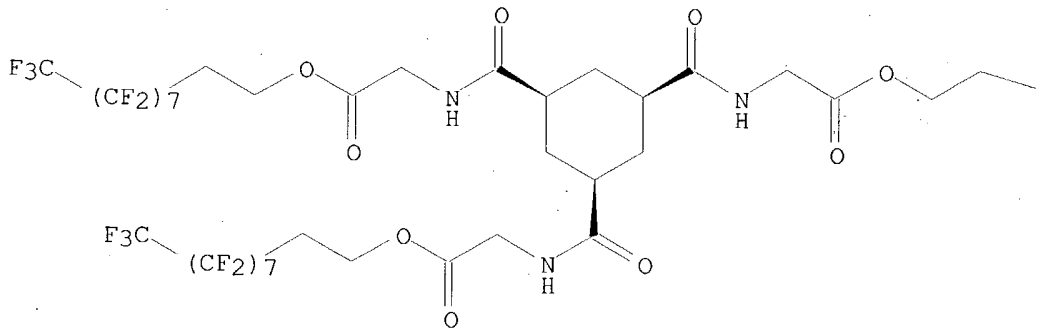
IT **277750-49-9P 277756-64-6P**
RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(assocn. of compds. in carbon dioxide and gels and/or microcellular foams therefrom for fracturing subterranean formations)

RN 277750-49-9 HCAPLUS

CN Glycine, N,N',N''-[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-cyclohexanetriyltricarbonyl]tris-, tris(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl) ester (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:30681
GI

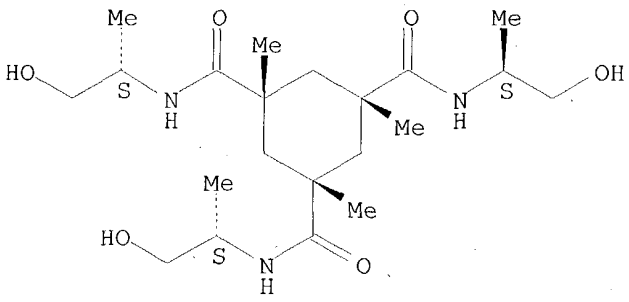
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Kemp's triacid was elaborated to optically pure tris(.beta.-hydroxylamide)s, e.g. I, and tris(oxazoline)s, e.g. II. The resulting C3-sym. compds. were used in diethylzinc addns. to benzaldehyde and allylic oxidns. of cyclopentene, based on Kharash reaction conditions, to give the corresponding products in good chem. yields and moderate enantioselectivities.

IT **273722-21-7P**
RL: CAT (Catalyst use); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(stereoselective prepn. of C3-sym. tris(carboxamide)s and tris(oxazoline)s from Kemp's acid as chiral ligands in asym. addn. and allylic oxidn. reactions)

RN 273722-21-7 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris[(1S)-2-hydroxy-1-methylethyl]-1,3,5-trimethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

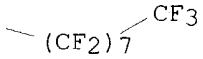


IT **273722-22-8P**
RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(stereoselective prepn. of C3-sym. tris(carboxamide)s and tris(oxazoline)s from Kemp's acid as chiral ligands in asym. addn. and allylic oxidn. reactions)

RN 273722-22-8 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris[(1S)-1-(hydroxymethyl)-2-methylpropyl]-1,3,5-trimethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

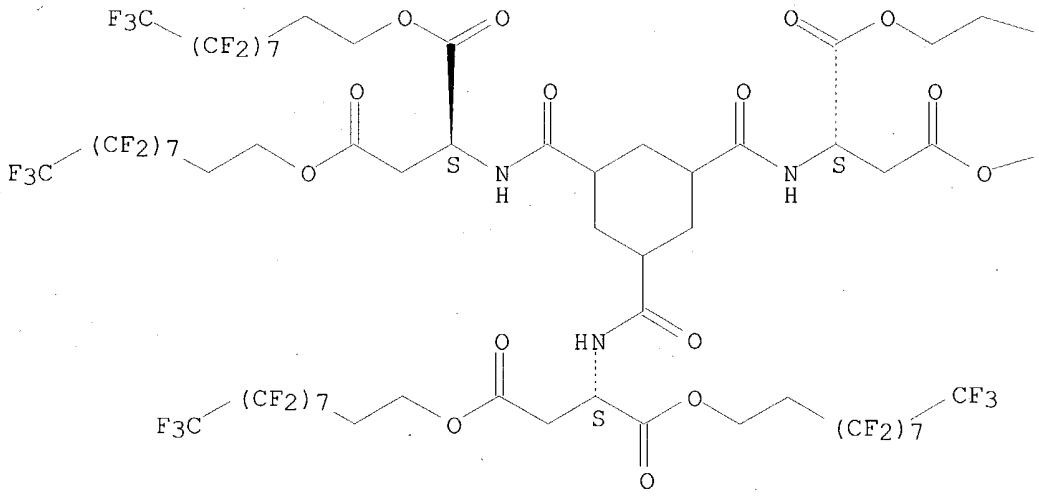
PAGE 1-B



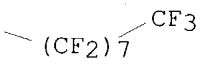
RN 277756-64-6 HCAPLUS
CN Butanedioic acid, 2,2',2''-[1,3,5-cyclohexanetriyltris(carbonylimino)]tris-, hexakis(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl) ester, (2S,2'S,2''S)- (9CI) (CA INDEX NAME)

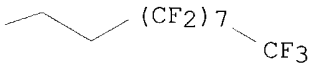
Absolute stereochemistry.

PAGE 1-A

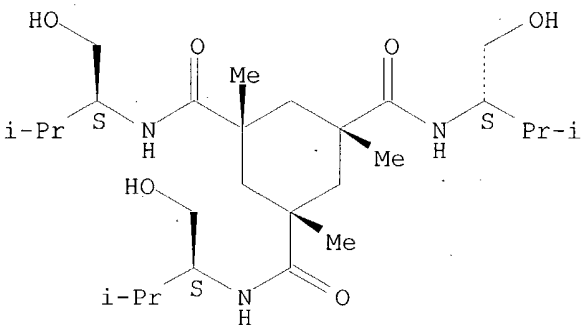


PAGE 1-B



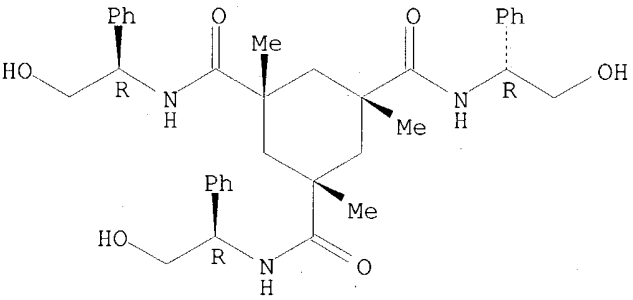


L27 ANSWER 23 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:251206 HCAPLUS
DOCUMENT NUMBER: 133:30681
TITLE: Preparation and catalytic enantioselective reactions of C3-symmetric tris(oxazoline)s derived from Kemp's triacid
AUTHOR(S): Chuang, Tsung-Hsun; Fang, Jim-Min; Bolm, Carsten
CORPORATE SOURCE: Department of Chemistry, National Taiwan University, Taipei, 106, Taiwan
SOURCE: Synthetic Communications (2000), 30(9), 1627-1641
CODEN: SYNCAV; ISSN: 0039-7911
PUBLISHER: Marcel Dekker, Inc.



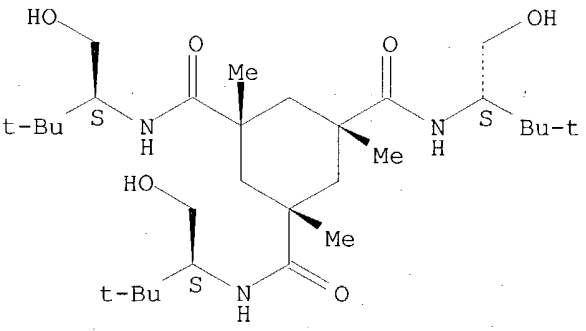
IT **273722-20-6P 273722-23-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(stereoselective prepn. of C3-sym. tris(carboxamide)s and tris(oxazoline)s from Kemp's acid as chiral ligands in asym. addn. and allylic oxidn. reactions)
RN 273722-20-6 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris[(1R)-2-hydroxy-1-phenylethyl]-1,3,5-trimethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 273722-23-9 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris[(1S)-1-(hydroxymethyl)-2,2-dimethylpropyl]-1,3,5-trimethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 95 THERE ARE 95 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 24 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:705529 HCAPLUS
DOCUMENT NUMBER: 132:108275
TITLE: Thermodynamics of Formation of the Triple Helix from Free Chains and from Template-Constrained Chains of Collagen-like Monodisperse Poly(Gly-Pro-Hyp) Structures
AUTHOR(S): Locardi, Elsa; Kwak, Juliann; Scheraga, Harold A.; Goodman, Murray
CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of California at San Diego, La Jolla, CA, 92093-0343, USA
SOURCE: Journal of Physical Chemistry A (1999), 103(49), 10561-10566
CODEN: JPCAFH; ISSN: 1089-5639
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

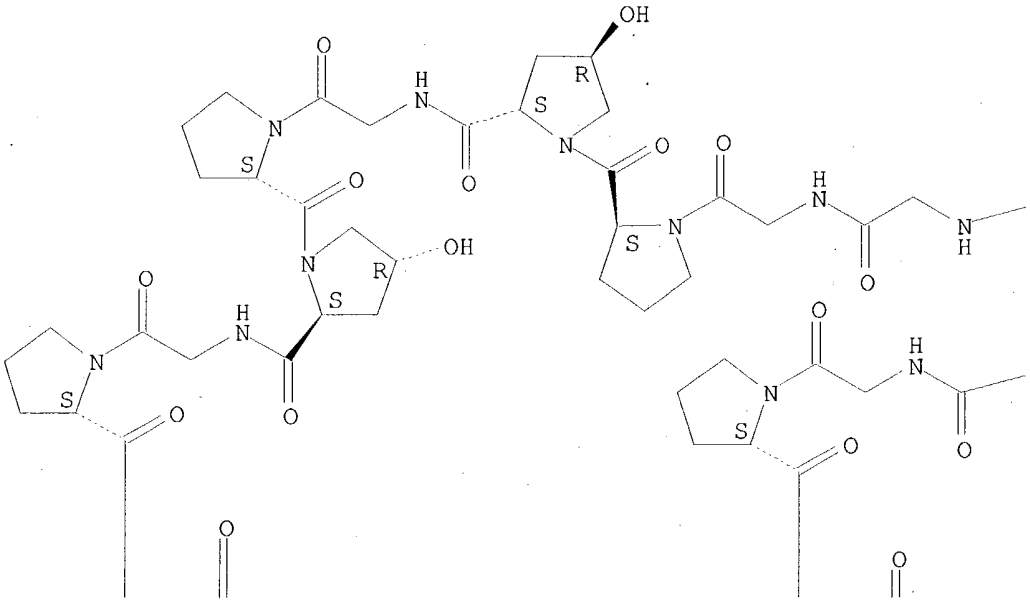
AB Statistical thermodn. methods, developed for treating the .alpha.-helix-coil transition, are applied herein to describe the formation of the triple helix from short free chains and short template-constrained chains of collagen-like monodisperse poly(tripeptides), using poly(Gly-Pro-Hyp) as the example. For such short chains, application of the one-helical-sequence approxn. indicates that there is very little unwinding from the ends, so that an all-or-none model is adequate to treat this transition. From the dependence of the helix nucleation and propagation parameters on chain length, concn., and temp., the thermodn. parameters for formation of the triple helix from both free chains and template-constrained monodisperse poly(Gly-Pro-Hyp) chains are similar, and also similar to those for free poly(Gly-Pro-Pro) chains.

IT **176839-96-6**
RL: PRP (Properties)
(thermodn. of formation of the triple helix from free chains and from template-constrained chains of monodisperse poly(Gly-Pro-Hyp) structures)

RN 176839-96-6 HCAPLUS
CN L-Prolinamide, 1,1',1''-[[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-trimethyl-1,3,5-cyclohexanetriyl]tricarbonyl]tris[glycylglycyl-L-prolyl-(4R)-4-hydroxy-L-prolylglycyl-L-prolyl-(4R)-4-hydroxy-L-prolylglycyl-L-prolyl-4-hydroxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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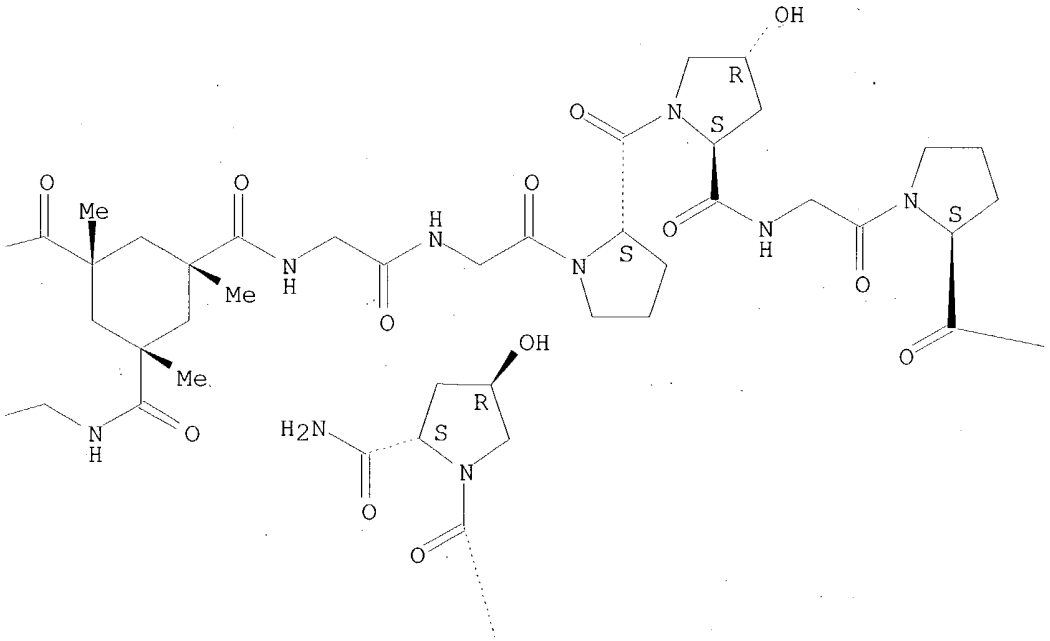
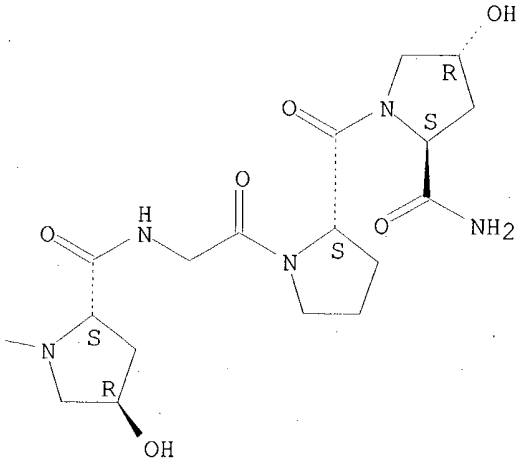
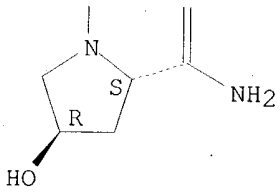


PAGE 1-C





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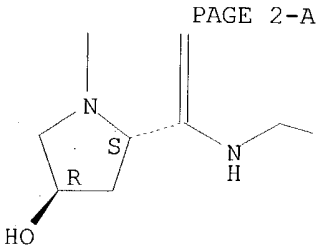

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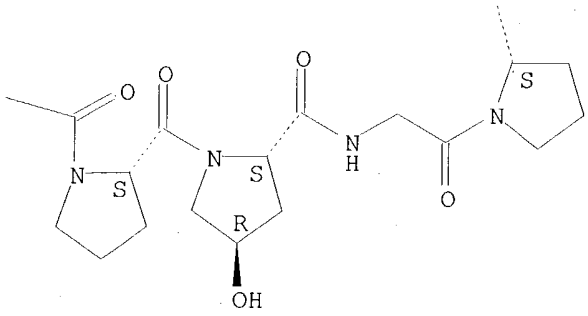


REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 25 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:559232 HCAPLUS
DOCUMENT NUMBER: 131:316063
TITLE: Supramolecular liquid-crystalline materials formed by hydrogen-bonded assembly processes
AUTHOR(S): Kato, Takashi; Yasuda, Takayasu; Kanie, Kiyoshi; Ihata, Osamu; Mizoshita, Norihiro; Hanabusa, Kenji; Ukon, Masakatsu; Shimizu, Yo
CORPORATE SOURCE: Department of Chemistry and Biotechnology, School of Engineering, The University of Tokyo, Tokyo, 113-8656,

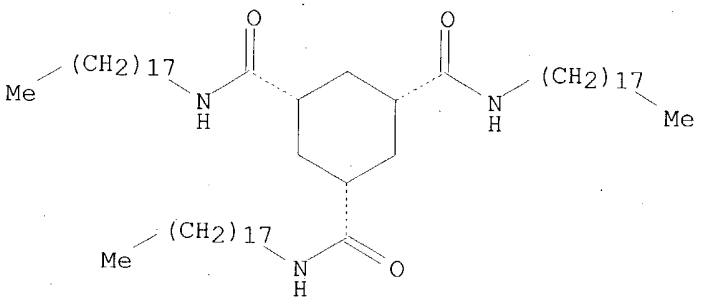
Japan
SOURCE: Polymer Preprints (American Chemical Society, Division of Polymer Chemistry) (1999), 40(2), 1104-1105
CODEN: ACPPAY; ISSN: 0032-3934
PUBLISHER: American Chemical Society, Division of Polymer Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Hydrogen-bonded mesogenic complexes are of 2 types: identical mols. and different mols. Dialkoxyphenyl moieties were incorporated into the glutamic acid unit of folic acid. These derivs. exhibit thermotropic mesomorphic properties due to the hydrogen-bonded tetramer formation. Hydrogen-bonded complexes of 2,6-bis(acylamino)pyridine and 4-alkoxybenzoic acid exhibit various liq. crystal phases. The formation of anisotropic composites of gelling agents and nematic, smectic and discotic liq. crystals with well-organized structures is described.

IT **189299-30-7**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(hydrogen-bonded assembly of gelling agents in triphenylene deriv. discotic liq. crystal)

RN 189299-30-7 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-trioctadecyl-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 26 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:444485 HCAPLUS
DOCUMENT NUMBER: 131:157896
TITLE: Synthesis of simple multivalent .beta.-D-GalNAc-(1.fwdarw.4)-.beta.-D-Gal oligomers as probes for investigating the interactions of P. aeruginosa pili with multivalent receptors
AUTHOR(S): Jiao, Hailong; Hindsgaul, Ole
CORPORATE SOURCE: Department of Chemistry, University of Alberta, Edmonton, AB, T6G 2G2, Can.
SOURCE: Journal of Carbohydrate Chemistry (1999), 18(5), 499-513
CODEN: JCACDM; ISSN: 0732-8303
PUBLISHER: Marcel Dekker, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Five multivalent .beta.-D-GalNAc-(1.fwdarw.4)-.beta.-D-Gal oligomers were selected and synthesized as probes for investigating the adhesin-receptor interactions of P. aeruginosa pill with multivalent receptors. They were synthesized by the amide coupling reactions of 8-(N-2-

aminoethyl)carboxamidooctyl 4-O-(2-acetamido-2-deoxy-.beta.-D-galactopyranosyl)-.beta.-D-galactopyranoside (1) with EDTA dianhydride, EDTA, Kemp's triacid and adipic acid with EDC, DIC and DCC combined with HOBt as coupling reagents and by the reaction of per-O-acetylated 1 with 1,3,5-benzenetricarbonyl trichloride followed by de-O-acetylation. These resulting multivalent compds. contain flexible C9 spacer arms as linkers attached to either flexible hydrophilic moieties or rigid hydrophobic cores.

IT **236743-67-2P**

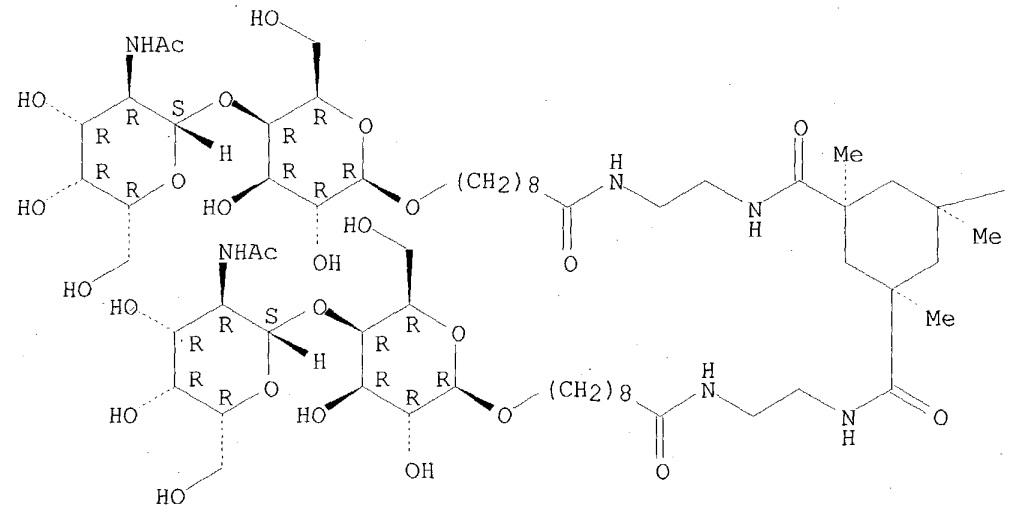
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of simple multivalent oligosaccharides as probes for investigating the interactions of P. aeruginosa pili with multivalent receptors)

RN 236743-67-2 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris[2-[[9-[[4-O-[2-(acetylamino)-2-deoxy-.beta.-D-galactopyranosyl]-.beta.-D-galactopyranosyl]oxy]-1-oxononyl]amino]ethyl]-1,3,5-trimethyl-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A



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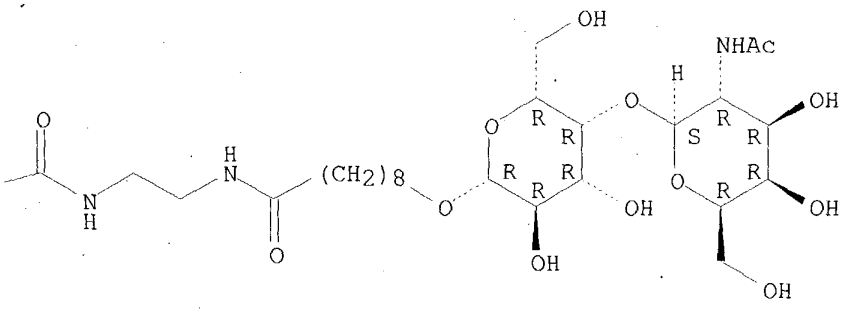


REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 27 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:427215 HCAPLUS
DOCUMENT NUMBER: 131:90194
TITLE: Photoelectric converters and photoelectrochemical cells thereof
INVENTOR(S): Shirato, Kentaro; Yanagida, Shozo; Shirai, Hiroyoshi; Hanabusa, Kenji
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 39 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11185836	A2	19990709	JP 1997-363503	19971216

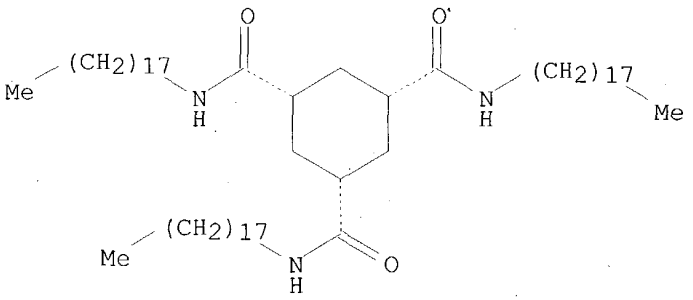
PRIORITY APPLN. INFO.: JP 1997-363503 19971216

AB The photoelec. converters have a conductive substrate, a layer of semiconductor particles contg. adsorbed dye on the substrate, a gel electrolyte, and a counter electrode; where the gel electrolyte contains an electrolyte and a gelling agent having mol. wt. .ltoreq.1000. The salts are selected from metal iodide, quaternary ammonium iodide, quaternary imidazolium iodide, quaternary pyridinium iodide, metal bromide, quaternary ammonium bromide, S compds., viologen dye, and hydroquinone-quinone.

IT **189299-30-7**
RL: DEV (Device component use); USES (Uses)
(electrolyte gelling agents for photoelectrochem. cells with dye adsorbed semiconductor electrodes)

RN 189299-30-7 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-trioctadecyl-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L27 ANSWER 28 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:198807 HCAPLUS
DOCUMENT NUMBER: 131:29032
TITLE: Design, synthesis and conformations of novel triple helical collagen mimetic structures
AUTHOR(S): Goodman, Murray; Kwak, Juliann
CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of California, La Jolla, CA, 92093-0343, USA
SOURCE: Proceedings - Indian Academy of Sciences, Chemical Sciences (1999), 111(1), 35-49
CODEN: PIAADM; ISSN: 0253-4134

PUBLISHER: Indian Academy of Sciences
DOCUMENT TYPE: Journal
LANGUAGE: English

AB We have synthesized collagen-like monodisperse structures. A series of single chain Ac-(Gly-Pro-Hyp)n-NH2 where n = 1, 3, 5, 6, 9 and template-assembled KTA-[Gly-(Gly-Pro-Hyp)n-NH2]3 analogs (n = 1, 3, 5, 6), where KTA is the Kemp triacid (cis-1,3,5-trimethyl cyclohexane-1,3,5-tricarboxylic acid), were assessed for triple helicity by CD, thermal denaturation and NMR spectroscopy. The KTA-based template induces a significant gain in free energy and reduces the crit. chain length for triple helix formation over the acyl terminated single chain structures. Our approach also includes the incorporation of the peptoid residue N-isobutylglycine into the design for novel collagen-like sequences. We have synthesized and characterized acetylated single chain and template-assembled analogs composed of Gly-Pro-Nleu and Gly-Nleu-Pro sequences. The achiral trimeric unit Gly-Nleu-Nleu was included as a guest sequence in a host structure such as Ac-(Gly-Pro-Hyp)3-(Gly-Nleu-Nleu)3-(Gly-Pro-Hyp)3-NH2 which retains triple helicity. A series of guest-host collagen mimetics composed of Gly-Nleu-Pro sequences as the host were synthesized and assessed for triple helicity. Guest sequences include Gly-Nleu-Nleu and Gly-Nx-Pro units, where Nx is the guest peptoid residue with alkyl and aralkyl side chains. We have continued to investigate functionalized template motifs and sequence variations. We are examg. the effects of functionalization and sequence variation on triple helical stabilities and mol. properties in order to design novel collagen-based biomaterials.

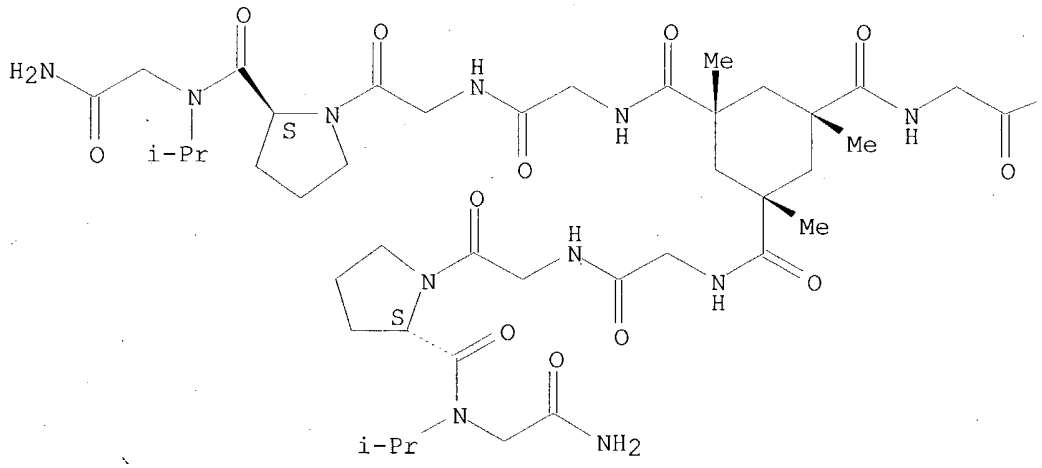
IT **226562-17-0 226562-18-1 226562-22-7**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(design, synthesis and conformations of novel triple helical collagen mimetic structures)

RN 226562-17-0 HCAPLUS

CN Glycinamide, 1,1',1''-[[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-trimethyl-1,3,5-cyclohexanetriyl]tricarbonyl]tris[glycylglycyl-L-prolyl-N2-(1-methylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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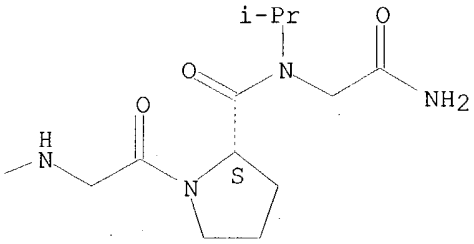
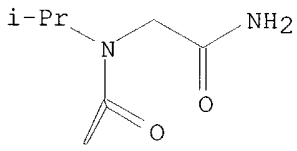
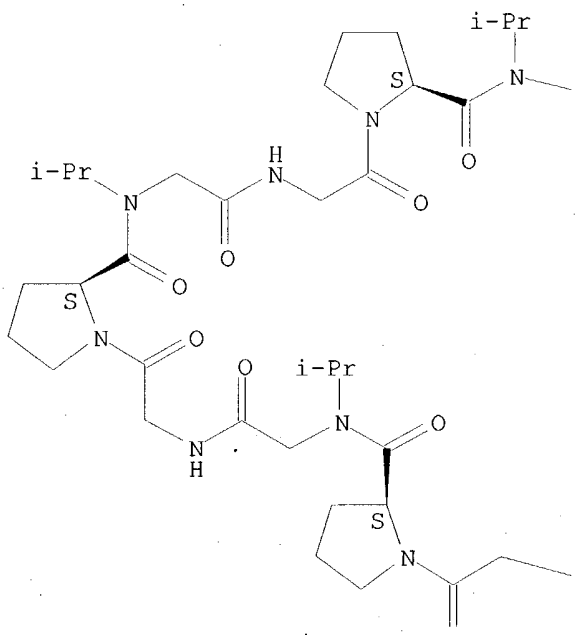


RN 226562-18-1 HCAPLUS
CN Glycinamide, 1,1',1''-[[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-trimethyl-1,3,5-cyclohexanetriyl]tricarbonyl]tris[glycylglycyl-L-prolyl-N-(1-methylethyl)glycylglycyl-L-prolyl-N-(1-methylethyl)glycylglycyl-L-prolyl-N2-(1-methylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A





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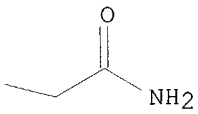

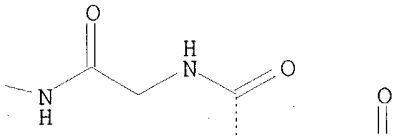

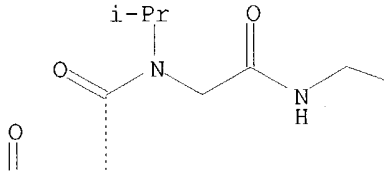

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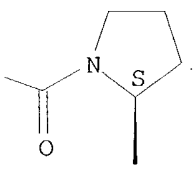

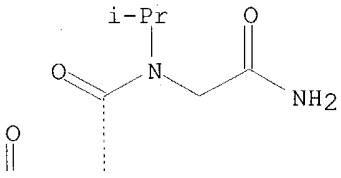

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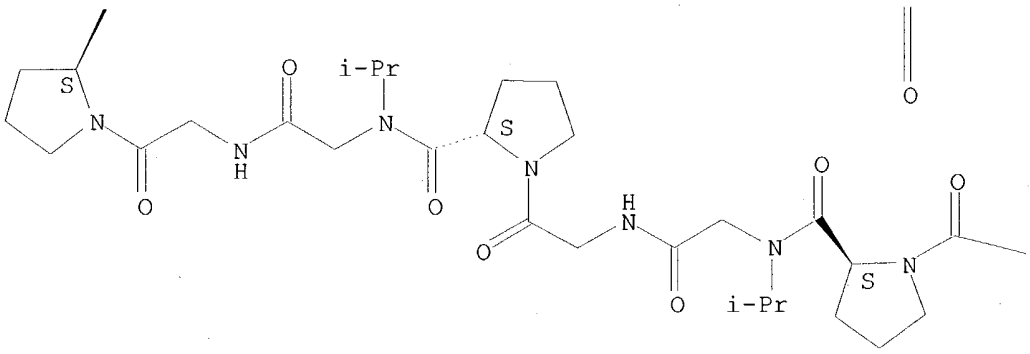

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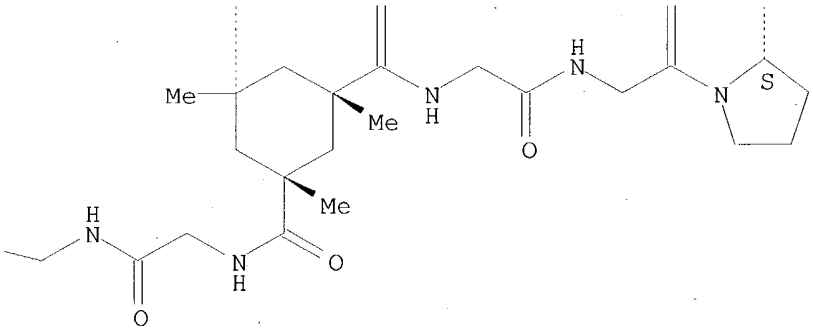

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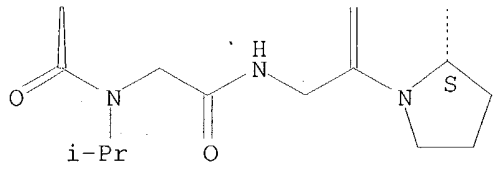
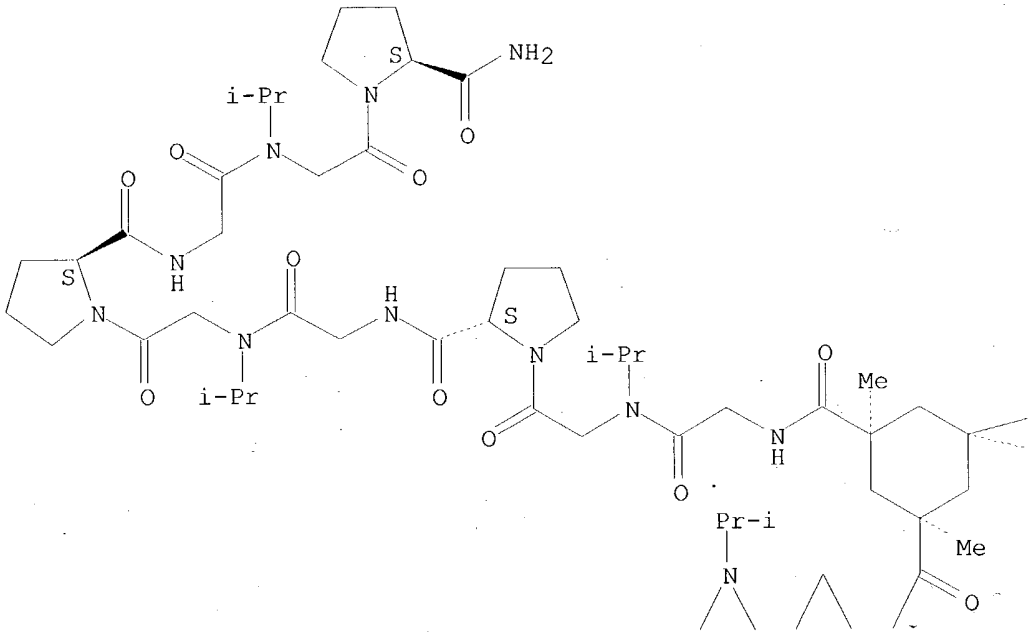


RN 226562-22-7 HCAPLUS
CN L-Prolinamide, 1,1',1''-[[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-trimethyl-1,3,5-cyclohexanetriyl]tricarbonyl]tris[glycyl-N-(1-methylethyl)glycyl-L-prolylglycyl-N-(1-methylethyl)glycyl-L-prolylglycyl-N-(1-methylethyl)glycyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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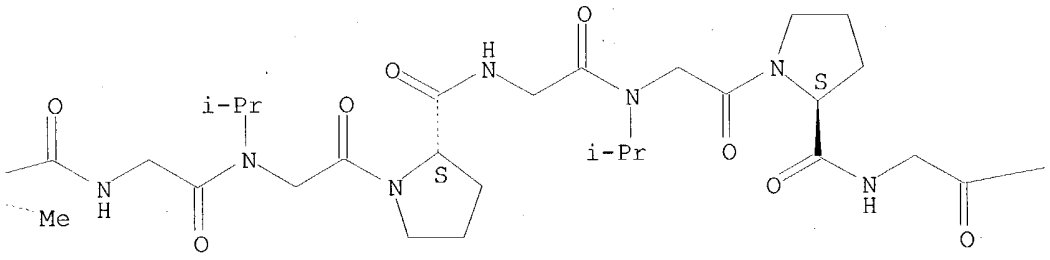

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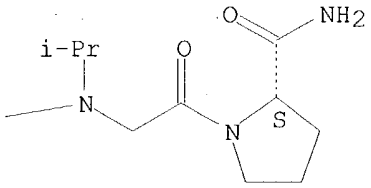
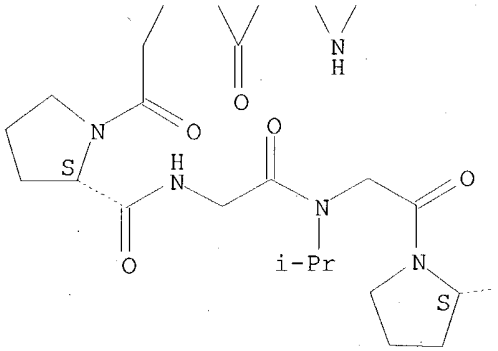


PAGE 2-A



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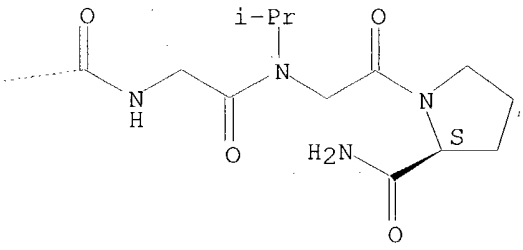


REFERENCE COUNT: 67 THERE ARE 67 CITED REFERENCES AVAILABLE FOR THIS

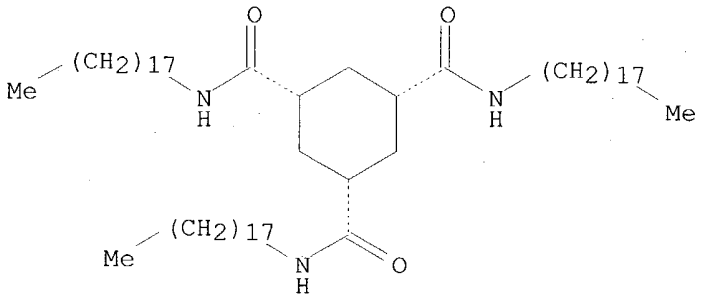
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 29 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:717725 HCAPLUS
DOCUMENT NUMBER: 130:4357
TITLE: Synthesis of low molecular weight organogelators and their physical gelation
AUTHOR(S): Hanabusa, Kenji; Shirai, Hirofusa
CORPORATE SOURCE: Department of Functional Polymer Science, Faculty of Textile Science and Technology, Shinshu University, Ueda, 386-8567, Japan
SOURCE: Kobunshi Ronbunshu (1998), 55(10), 585-594
CODEN: KBRBA3; ISSN: 0386-2186
PUBLISHER: Kobunshi Gakkai
DOCUMENT TYPE: Journal
LANGUAGE: Japanese

AB This article describes the low mol. wt. gelators which were reported since 1996. Alkylamides and alkylureas derived from trans-1,2-diaminocyclohexane are excellent organogelators which can gelate a wide variety of org. solvents, from protic polar solvents to aprotic non-polar ones. The results of gelation test of di-urea derivs. indicate that the intermol. hydrogen bonding between ureylene units is as very useful as the intermol. hydrogen bonding between amides for mol. design of gelators. Tridodecyl-1,3,5-benzenetricarboxamide is found to act as thickener, because the addn. of the small amt. of this compd. causes a marked rise of viscosity of hydrocarbons and oils. On the other hand, trioctadecyl-cis-1,3,5-cyclohexanetricarboxamide, which is structurally related to tridodecyl-1,3,5-benzenetricarboxamide, can cause phys. gelation of hydrocarbons and oils. Bolaform amides derived from L-valine or L-isoleucine are excellent organogelators for a wide variety of org. solvents, although they contain neither an arom. moiety nor a long methylene segment. The bolaform amides are expected to be smoothly-biodegradable organogelators. Besides the above gelators, this article deals with the following compds.; 4,4',4''-tris(stearoylamino)triphenylamine, an equimolar mixt. of isocyanuric acid and triaminopyrimidine contg. a cholesterol segment, .gamma.-alkoxybutyrolactone, quaternary ammonium halide salts, p-toluenesulfonic acid salt of L-leucine alkyl ester, fluoroalkylated oligomers, a 24-residue peptide, a biotin deriv., a cholic acid deriv., an N-alkylgluconamide deriv., and an L-isoleucine deriv.

IT **189299-30-7P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of low mol. wt. organogelators and their phys. gelation)
RN 189299-30-7 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-trioctadecyl-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

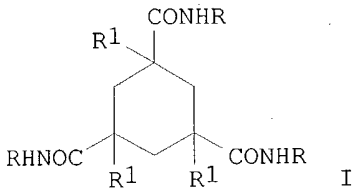
Relative stereochemistry.



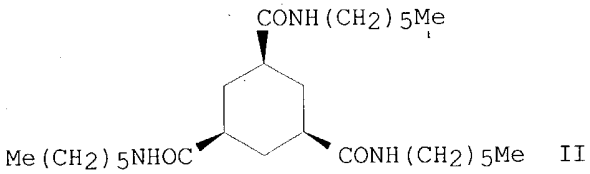
L27 ANSWER 30 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:665873 HCAPLUS
DOCUMENT NUMBER: 129:330490
TITLE: Preparation of cyclohexanetricarboxamide derivatives as thickening and/or gelation agents
INVENTOR(S): Hanabusa, Kenji; Kawakai, Atsushi; Shirai, Hiroyoshi; Iyanagi, Koichi
PATENT ASSIGNEE(S): Pola Chemical Industries, Inc., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 10273477	A2	19981013	JP 1997-344691	19971215
JP 3500289	B2	20040223		

PRIORITY APPLN. INFO.: JP 1997-29790 A 19970129
OTHER SOURCE(S): MARPAT 129:330490
GI



I



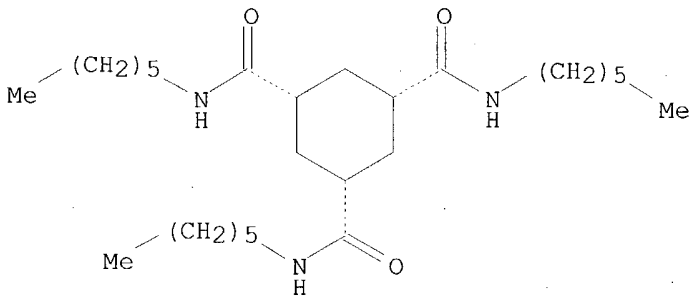
II

AB The title compds. (I; R = C4-20 linear or branched alkyl; R1 = H, C1-4 alkyl), which provide thickening and/or gelation or stabilization means for fluid org. compds. or compns. contg. them, are prepd. Thus, cis-1,3,5-cyclohexanetri(carboxylic acid) was dissolved in CHCl3, treated with SOCl2, stirred at room temp. for 1 h, and concd., and then condensed with hexylamine in the presence of Et3N in CH2Cl2 under heating to give the title compd. (II). II (3 mg) was added to 1 cm3 pyridine, heated to 100.degree., and cooled to give a gel.

IT **189299-28-3P 189299-29-4P 189299-30-7P 189301-40-4P 215231-39-3P**
RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(prepn. of cyclohexanetricarboxamide derivs. as thickening and/or gelation agents)

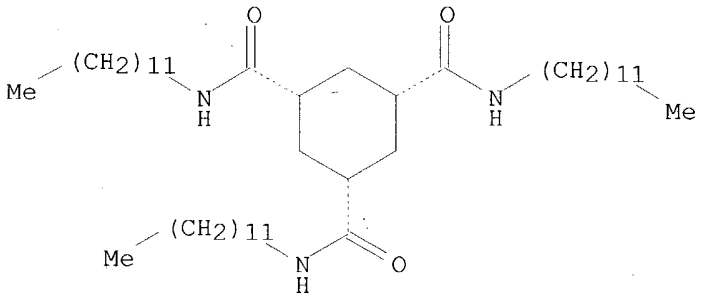
RN 189299-28-3 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-trihexyl-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



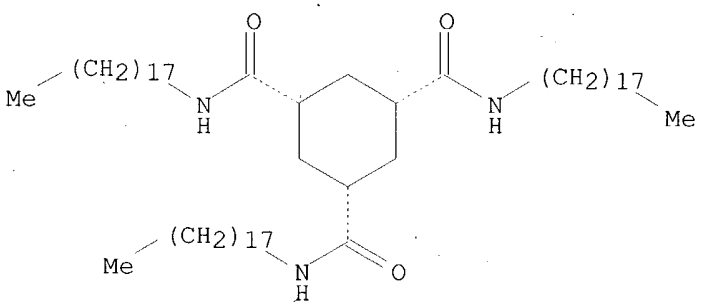
RN 189299-29-4 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tridodecyl-,
(1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 189299-30-7 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-trioctadecyl-,
(1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

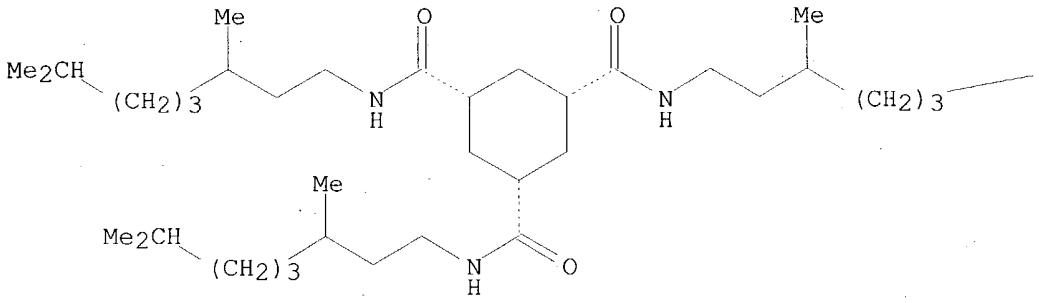
Relative stereochemistry.



RN 189301-40-4 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris(3,7-dimethyloctyl)-,
(1.alpha.,3.alpha.,5.alpha.)-[partial]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



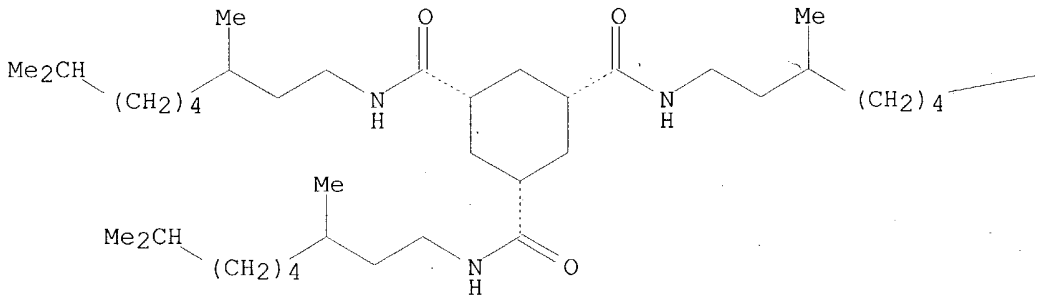
PAGE 1-B

—CHMe2

RN 215231-39-3 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris(3,8-dimethylnonyl)-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



PAGE 1-B

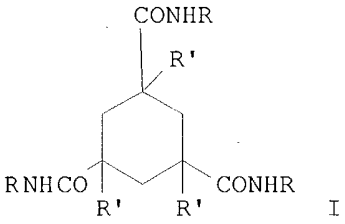
—CHMe2

L27 ANSWER 31 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:512440 HCAPLUS
DOCUMENT NUMBER: 129:221032
TITLE: Cosmetic, pharmaceutical, or food compositions containing cyclohexanetricarboxamides as thickening agents
INVENTOR(S): Hide, Kenji; Kawaue, Atsushi; Shirai, Hirofusa; Iyanagi, Koichi
PATENT ASSIGNEE(S): Pola Chemical Industries, Inc., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.
CODEN: JKXXAF

DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 10212213	A2	19980811	JP 1997-29602	19970129
JP 3501612	B2	20040302		

PRIORITY APPLN. INFO.: JP 1997-29602 19970129
OTHER SOURCE(S): MARPAT 129:221032
GI



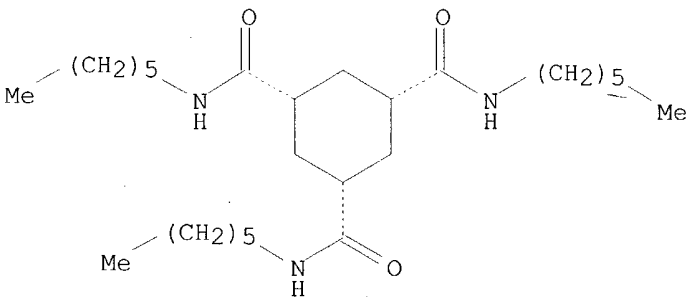
I

AB Title compns. contain cyclohexanetricarboxamides I (R = C4-20 alkyl; R' = H, C1-4 alkyl) as thickening or gelation agents. The compns. are stable at high temp. (.apprx.40.degree.). A foundation was prepd. from glyceryl triisooctanate 10, jojoba oil 10, dimethicone 10, carnauba wax 10, cis-I (R = hexyl, R' = H) (prepn. given) 1, mica 19, talc 10, TiO2 10, yellow iron oxide 5, red iron oxide 2, and nylon powder 13 parts.

IT **189299-28-3P 189299-29-4P 189299-30-7P**
189301-40-4P 212268-42-3P 212268-43-4P
RL: BUU (Biological use, unclassified); FFD (Food or feed use); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(cyclohexanetricarboxamides as thickening or gelation agents for cosmetics, pharmaceuticals, and foods)

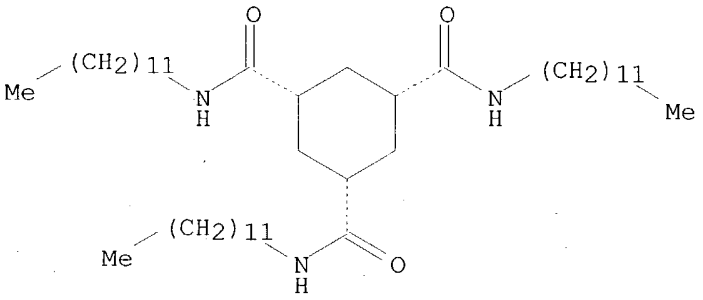
RN 189299-28-3 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-trihexyl-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



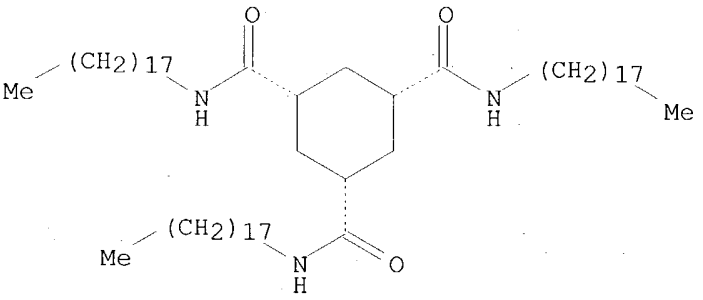
RN 189299-29-4 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tridodecyl-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 189299-30-7 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-trioctadecyl-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

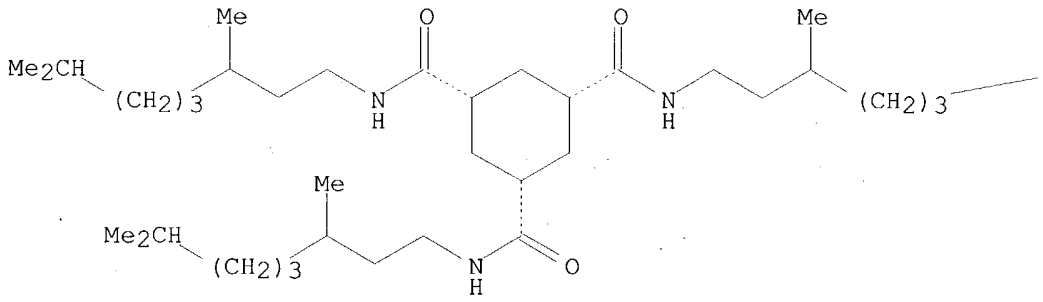
Relative stereochemistry.



RN 189301-40-4 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris(3,7-dimethyloctyl)-, (1.alpha.,3.alpha.,5.alpha.)-[partial]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A

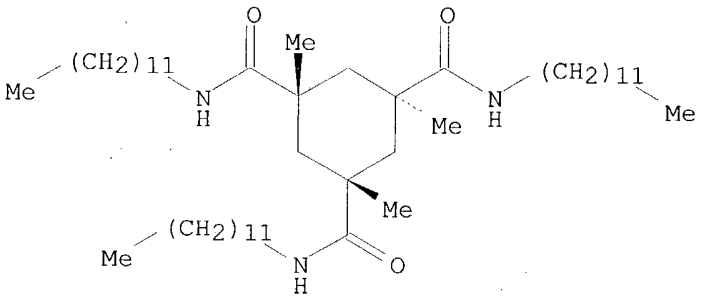


PAGE 1-B

—CHMe2

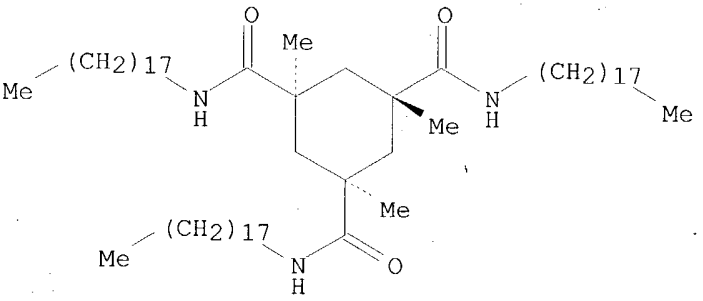
RN 212268-42-3 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tridodecyl-1,3,5-trimethyl-, (1.alpha.,3.alpha.,5.beta.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 212268-43-4 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, 1,3,5-trimethyl-N,N',N''-trioctadecyl-, (1.alpha.,3.alpha.,5.beta.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L27 ANSWER 32 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:496607 HCAPLUS
DOCUMENT NUMBER: 129:245455
TITLE: Incorporation of Achiral Peptoid-Based Trimeric Sequences into Collagen Mimetics
AUTHOR(S): Jefferson, Elizabeth A.; Locardi, Elsa; Goodman, Murray
CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of California San Diego, La Jolla, CA, 92093-0343, USA
SOURCE: Journal of the American Chemical Society (1998), 120(30), 7420-7428
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB This report represents initial studies of collagen mimetics with achiral peptoid-based trimeric sequences. The incorporation of achiral units into collagen-like structures is of considerable interest for the structural simplification of collagen-like biomaterials. The achiral unit Gly-Nleu-Nleu (Nleu = N-isobutylglycine) was positioned between Gly-Pro-Hyp trimeric repeats in collagen-like structures in order to examine the effect of an achiral block on triple helicity. A series of single chain structures, Ac-(Gly-Pro-Hyp)n-(Gly-Nleu-Nleu)n-(Gly-Pro-Hyp)n-NH2 (n = 1-3), and a template-assembled structure, KTA-[Gly-(Gly-Pro-Hyp)2-(Gly-Nleu-Nleu)2-(Gly-Pro-Hyp)2-NH2]3 (KTA = cis,cis-1,3,5-trimethylcyclohexane-1,3,5-tricarboxylic acid), were investigated. Biophys. studies were carried out in both H2O and ethylene glycol (EG)/H2O

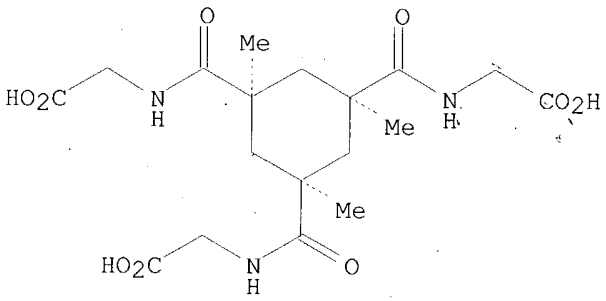
(2:1, vol./vol.) solvents, using CD and optical rotation measurements. Highly cooperative melting curves from optical rotation detns. were obtained for Ac-(Gly-Pro-Hyp)n-(Gly-Nleu-Nleu)n-(Gly-Pro-Hyp)n-NH2 (n = 2, 3) and KTA-[Gly-(Gly-Pro-Hyp)2-(Gly-Nleu-Nleu)2-(Gly-Pro-Hyp)2-NH2]3, revealing that the achiral trimer can participate in triple helical structures. These results were also supported by CD spectroscopy. For the mols. Ac-(Gly-Pro-Hyp)3-(Gly-Nleu-Nleu)3-(Gly-Pro-Hyp)3-NH2 and KTA-[Gly-(Gly-Pro-Hyp)2-(Gly-Nleu-Nleu)2-(Gly-Pro-Hyp)2-NH2]3, the presence of collagen-like structures was also supported by 1H NMR spectroscopy in H2O. For each structure, a distinct set of resonances, obtained at low temp., disappeared once a thermal denaturation temp. was reached. Furthermore, the anal. of NOE cross-peaks established the close packing of Pro, Hyp, and Nleu. The spatial proximity of Pro and Nleu residues and of Hyp and Nleu residues belonging to different chains was confirmed by mol. modeling of triple helical Ac-(Gly-Pro-Hyp)3-(Gly-Nleu-Nleu)3-(Gly-Pro-Hyp)3-NH2.

IT **183888-51-9**
RL: RCT (Reactant); RACT (Reactant or reagent)
(incorporation of achiral peptoid-based trimeric sequences into collagen mimetics)

RN 183888-51-9 HCAPLUS

CN Glycine, N,N',N''-[[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-trimethyl-1,3,5-cyclohexanetriyl]tricarbonyl]tris- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 33 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1998:233900 HCAPLUS

DOCUMENT NUMBER: 129:149208

TITLE: The activated core approach to combinatorial chemistry: a selection of new core molecules

AUTHOR(S): Pryor, Kent E.; Shipps, W., Jr.; Skyler, David A.; Rebek, Julius, Jr.

CORPORATE SOURCE: Skaggs Institute for Chemical Biology and Department of Chemistry, The Scripps Research Institute, La Jolla, CA, 92037, USA

SOURCE: Tetrahedron (1998), 54(16), 4107-4124
CODEN: TETRAB; ISSN: 0040-4020

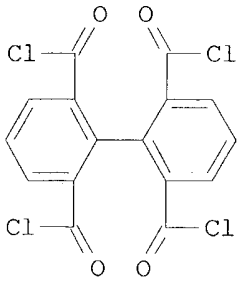
PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

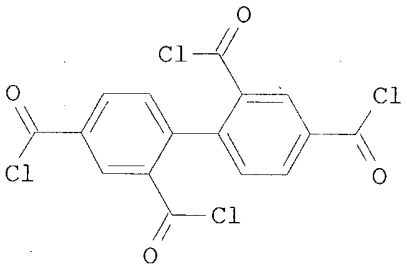
LANGUAGE: English

OTHER SOURCE(S): CASREACT 129:149208

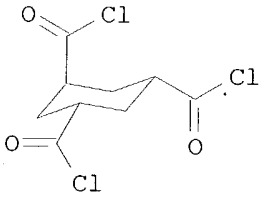
GI



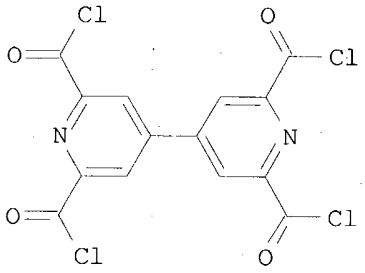
I



II



III



IV

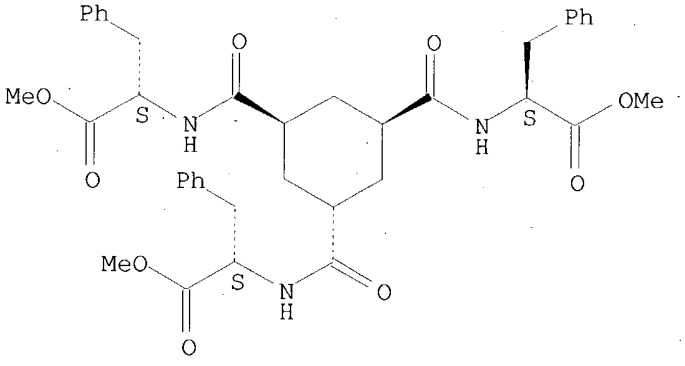
AB Four new activated core mols. I-IV, suitable for use in soln.-phase combinatorial org. chem. have been prepd. These mols. represent an attempt to further explore shape-space and increase the structural diversity of prepd. libraries, as well as to incorporate recognition elements in the cores to increase the chances for interaction with biol. targets. Demonstrations of deconvolution strategies used to simplify complex libraries and build individual mol. species based on the cores are also provided.

IT **206647-41-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of activated core mols. for prepn. of combinatorial libraries)

RN 206647-41-8 HCAPLUS

CN L-Phenylalanine, N,N',N''-[(1.alpha.,3.alpha.,5.beta.)-1,3,5-cyclohexanetriyltricarbonyl]tris-, trimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



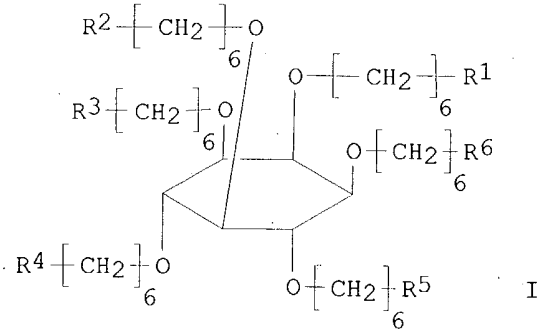
REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 34 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:31317 HCAPLUS

DOCUMENT NUMBER: 128:102343
TITLE: Preparation and uses of saccharide-containing dendrimers with a cyclohexane-polyol or inositol core.
INVENTOR(S): Wiessler, Manfred; Gschrey, Markus; Von der Lieth, Willi; Mier, Walter
PATENT ASSIGNEE(S): Deutsches Krebsforschungszentrum Stiftung des Offentlichen Rechts, Germany; Wiessler, Manfred; Gschrey, Markus; Von der Lieth, Willi; Mier, Walter
SOURCE: PCT Int. Appl., 28 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9748711	A1	19971224	WO 1997-DE1278	19970618
W: JP, US				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
DE 19624705	A1	19980108	DE 1996-19624705	19960620
EP 906325	A1	19990407	EP 1997-931626	19970618
R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, NL, SE				
JP 2000513342	T2	20001010	JP 1998-502095	19970618
US 6417339	B1	20020709	US 1999-202843	19990308

PRIORITY APPLN. INFO.: DE 1996-19624705 A 19960620
WO 1997-DE1278 W 19970618
OTHER SOURCE(S): CASREACT 128:102343
GI



I

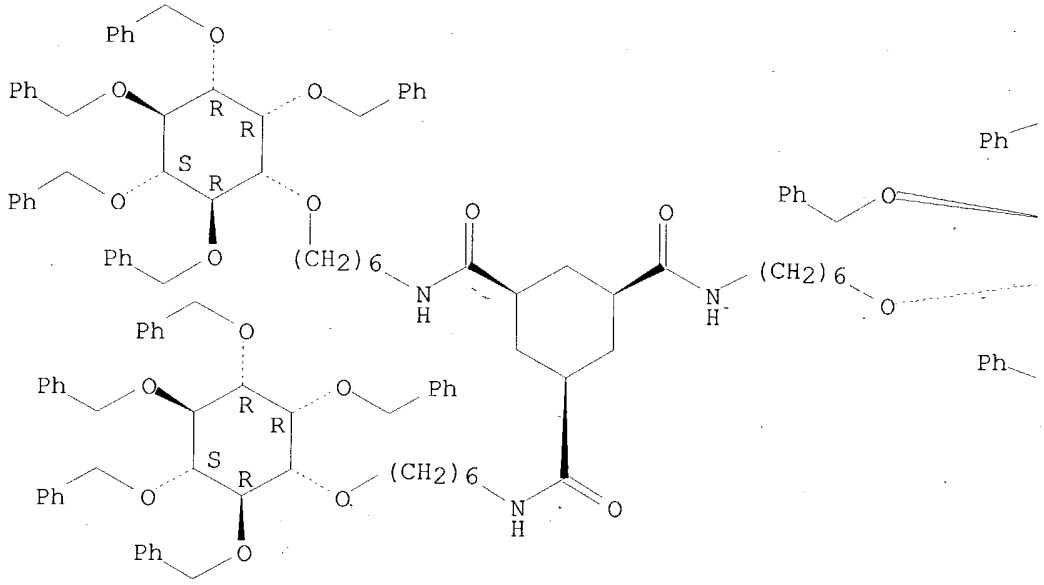
AB The invention relates to dendrimers comprising an initiator core with at least two functional groups and at least two saccharides. It also relates to the use thereof for various purposes e.g. as a catalyst in enantioselective synthesis, as a cellular adhesion inhibitor, as a carrier for medicinal agents or for purifn. of glycoproteins by affinity chromatog. Thus, 1,3,4,5,6-penta-O-benzyl-myo-inositol was reacted with 1,6-dibromo-hexane, followed by deprotection and azidation, and coupled with 6-bromo-hexyl-2,3,4,6-tetra-O-benzyl-.beta.-D-glucopyranoside, to give [(I); R1 = N3; R2-R6 = 2,3,4,6-tetra-O-benzyl-.beta.-D-glucopyranoside]. Using I as a column-chromatog. packing, racemic thalidomide was resolved.

IT **200201-40-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and uses of saccharide contg. dendrimers with a cyclohexane-polyol or inositol core)

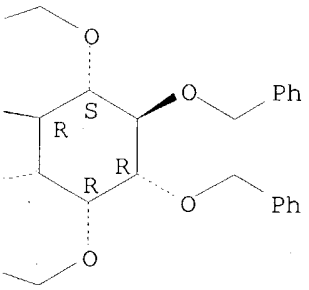
RN 200201-40-7 HCAPLUS
CN myo-Inositol, 3,3',3''-O-[[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-cyclohexanetriyl]tris(carbonylimino-6,1-hexanediyl)]bis[1,2,4,5,6-pentakis-O-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



L27 ANSWER 35 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1997:457086 HCAPLUS
DOCUMENT NUMBER: 127:81794
TITLE: Preparation of collagen-like peptoid residue-containing triple helical structures
INVENTOR(S): Goodman, Murray; Taulane, Joseph P.; Feng, Yangbo; Melacini, Giuseppe
PATENT ASSIGNEE(S): Regents of the University of California, USA
SOURCE: PCT Int. Appl., 57 pp.

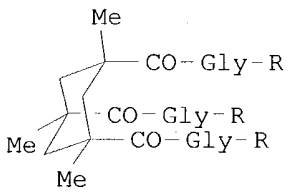
102(b)

CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9719106	A2	19970529	WO 1996-US18521	19961118
WO 9719106	A3	19970807		
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 6096710	A	20000801	US 1996-668380	19960621
CA 2237845	AA	19970529	CA 1996-2237845	19961118
AU 9710549	A1	19970611	AU 1997-10549	19961118
AU 716531	B2	20000224		
EP 861264	A2	19980902	EP 1996-941391	19961118
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 2000500497	T2	20000118	JP 1997-519839	19961118
US 6329506	B1	20011211	US 1999-388916	19990901
AU 750744	B2	20020725	AU 1999-65317	19991217
AU 9965317	A1	20000302		

PRIORITY APPLN. INFO.: US 1995-6894P P 19951117
US 1996-668380 A 19960621
WO 1996-US18521 W 19961118

OTHER SOURCE(S): MARPAT 127:81794
GI



I

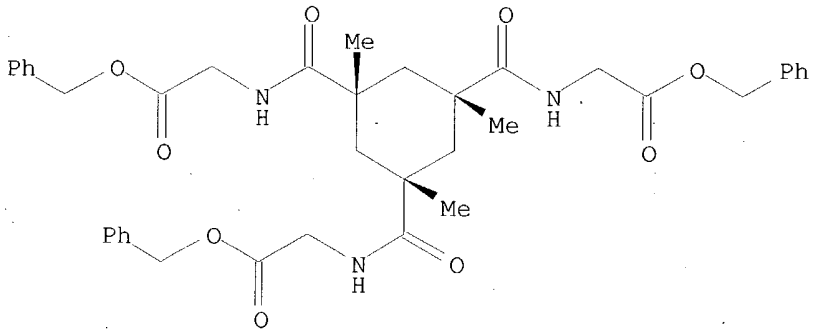
AB Synthetic collagen derivs. in triple helical conformation and comprising amino acid chains of repeating trimers Gly-Xp-Pro, Gly-Pro-Yp, Gly-Pro-Hyp, and Gly-Pro-Pro [Xp, Yp = N-substituted glycine (peptoid) residue] of highly populated collagen sequences are claimed. The invention includes methods of prepg. synthetic collagen structures having the triple helix conformation present in collagen from collagen-type polypeptides and poly(peptide-peptoid residue) chains by means of a helix-inducing template such as cis,cis-1,3,5-trimethyl-1,3,5-cyclohexanetricarboxylic acid (Kemp's triacid) and 1,3,5-benzenetricarboxylic acid. Thus, tripeptide sequence Boc-Gly-Pro-Hyp(CH2Ph)-MBHA resin was prepd., deprotected with 30% CF3CO2H in CH2Cl2, and coupled with Kemp triacid deriv. I (R = OH) in the presence of HOBt and diisopropylcarbodiimide, followed by resin cleavage and deprotection to give 56% collagen-like structure I (R = Gly-Pro-Hyp-NH2).

IT **183888-50-8P 183888-51-9P 191537-47-0P**
191537-48-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(prepn. of collagen-like peptoid residue-contg. triple helical structures)

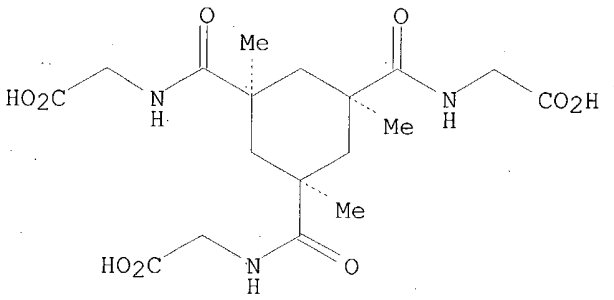
RN 183888-50-8 HCAPLUS
CN Glycine, N,N',N''-[[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-trimethyl-1,3,5-cyclohexanetriyl]tricarbonyl]tris-, tris(phenylmethyl) ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



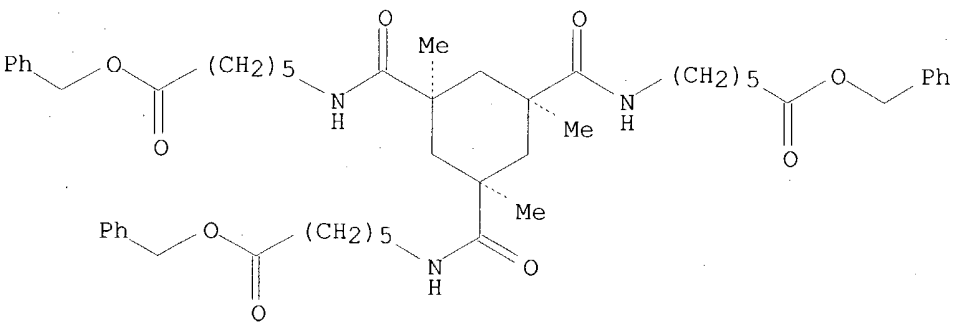
RN 183888-51-9 HCAPLUS
CN Glycine, N,N',N''-[[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-trimethyl-1,3,5-cyclohexanetriyl]tricarbonyl]tris- (9CI) (CA INDEX NAME)

Relative stereochemistry.



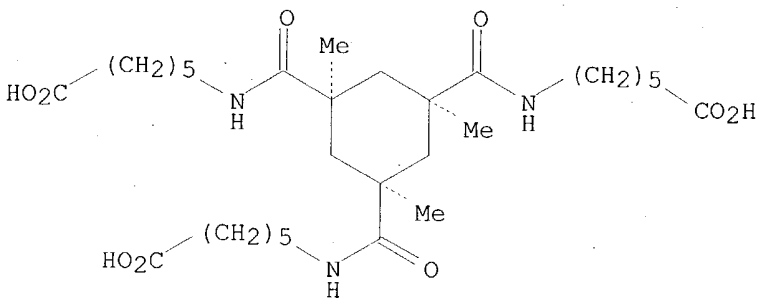
RN 191537-47-0 HCAPLUS
CN Hexanoic acid, 6,6',6''-[(1,3,5-trimethyl-1,3,5-cyclohexanetriyl)tris(carbonylimino)]tris-, tris(phenylmethyl) ester, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 191537-48-1 HCAPLUS
CN Hexanoic acid, 6,6',6''-[(1,3,5-trimethyl-1,3,5-cyclohexanetriyl)tris(carbonylimino)]tris-, (1.alpha.,3.alpha.,5.alpha.)-(9CI) (CA INDEX NAME)

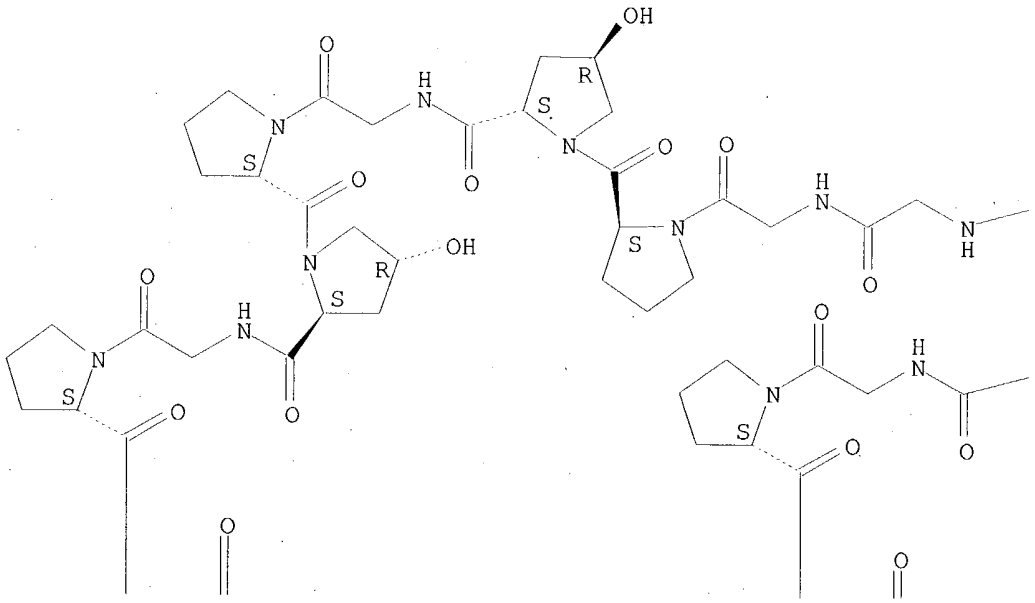
Relative stereochemistry.



IT **176839-96-6P 183888-57-5P 186031-88-9P 186031-89-0P 191537-50-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of collagen-like peptoid residue-contg. triple helical structures)
RN 176839-96-6 HCAPLUS
CN L-Prolinamide, 1,1',1''-[[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-trimethyl-1,3,5-cyclohexanetriyl]tricarbonyl]tris[glycylglycyl-L-prolyl-(4R)-4-hydroxy-L-prolylglycyl-L-prolyl-(4R)-4-hydroxy-L-prolylglycyl-L-prolyl-4-hydroxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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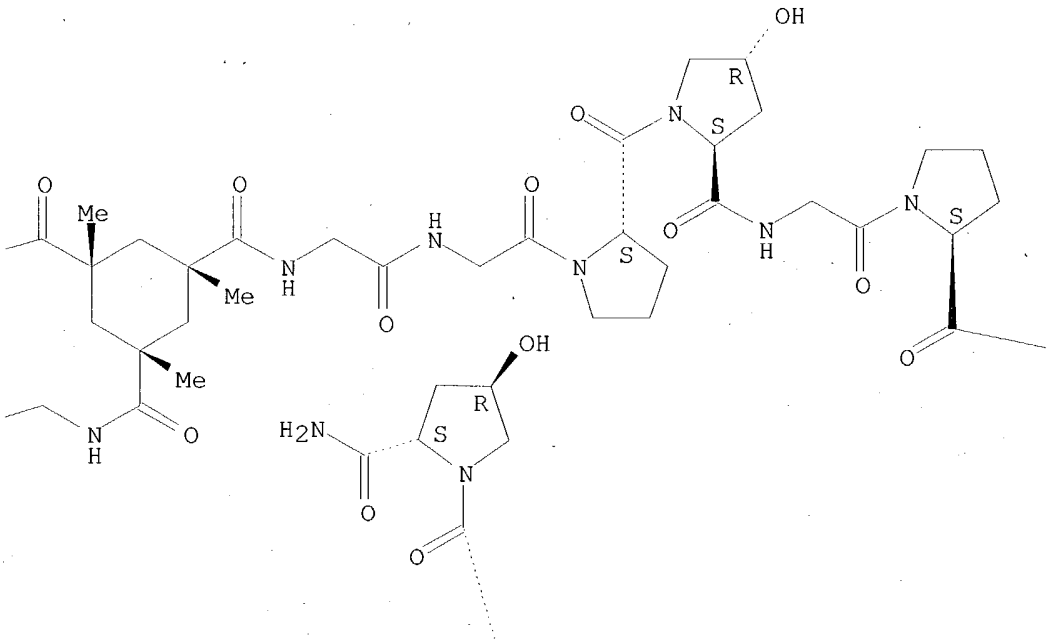

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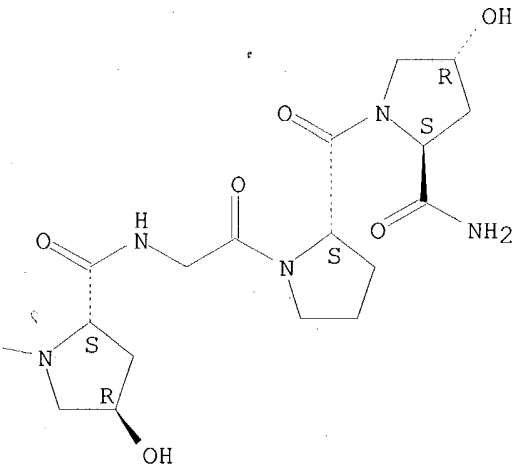

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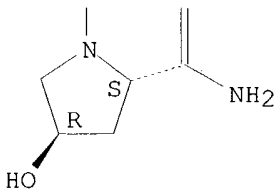

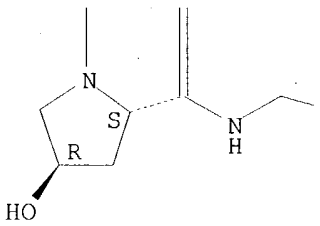

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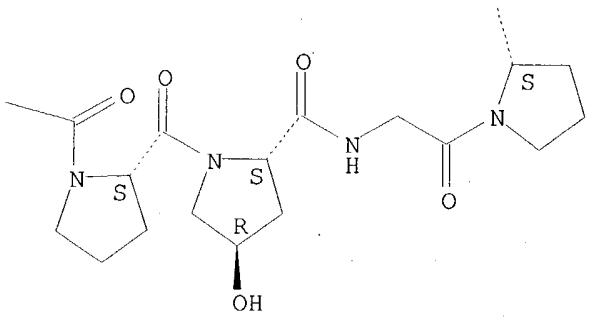
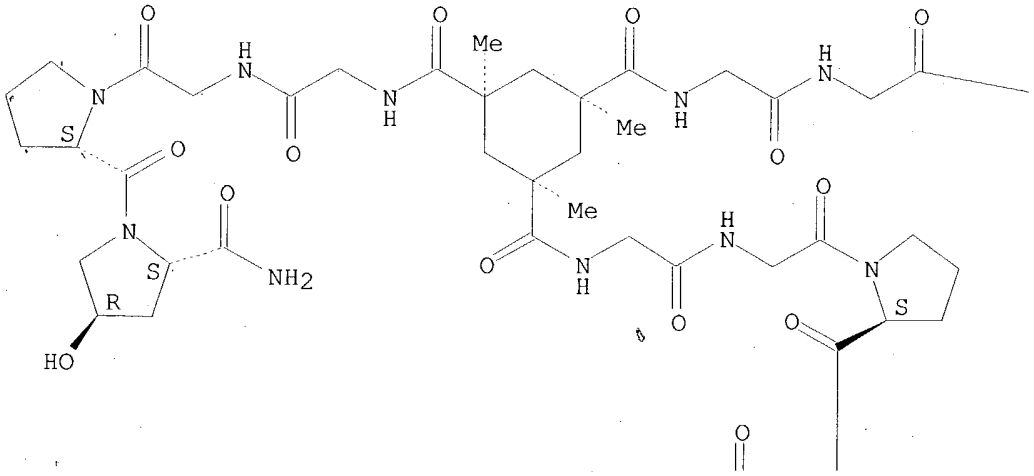


RN 183888-57-5 HCAPLUS
CN L-Prolinamide, 1,1',1''-[[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-trimethyl-1,3,5-cyclohexanetriyl]tricarbonyl]tris[glycylglycyl-L-prolyl-4-hydroxy-, (4R,4'R,4''R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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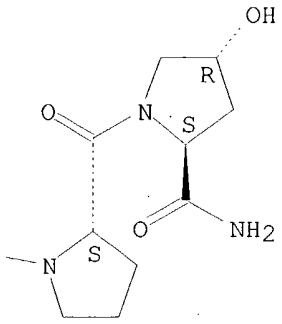

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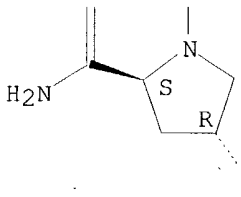
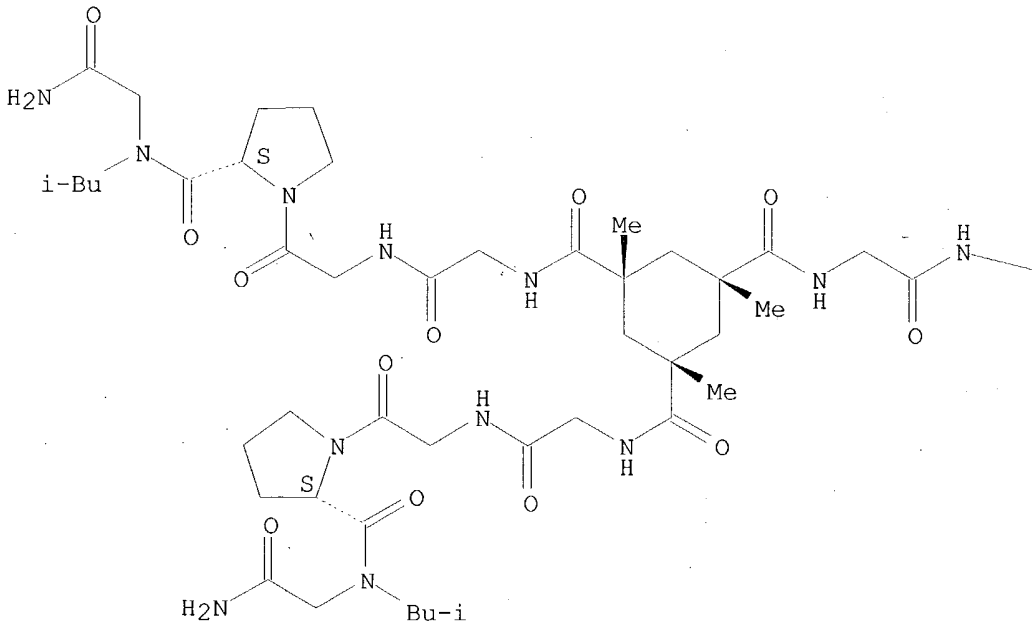


RN 186031-88-9 HCAPLUS
CN Glycinamide, 1,1',1''-[[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-trimethyl-1,3,5-cyclohexanetriyl]tricarbonyl]tris[glycylglycyl-L-prolyl-N2-(2-methylpropyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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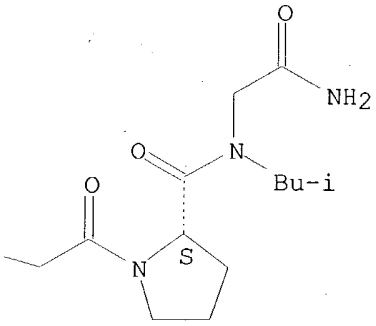
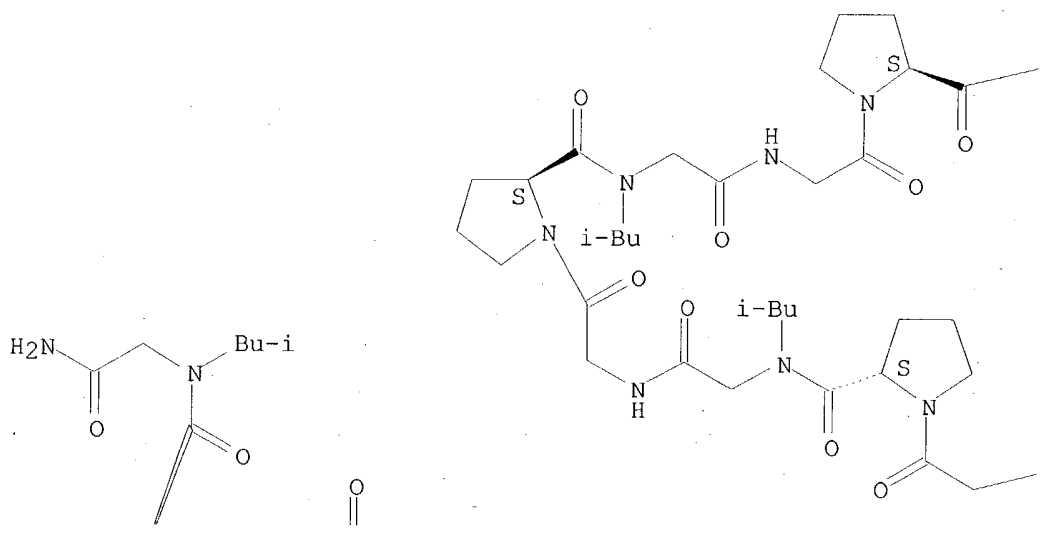


RN 186031-89-0 HCAPLUS
CN Glycinamide, 1,1',1''-[[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-trimethyl-1,3,5-cyclohexanetriyl]tricarbonyl]tris[glycylglycyl-L-prolyl-N-(2-methylpropyl)glycylglycyl-L-prolyl-N-(2-methylpropyl)glycylglycyl-L-prolyl-N2-(2-methylpropyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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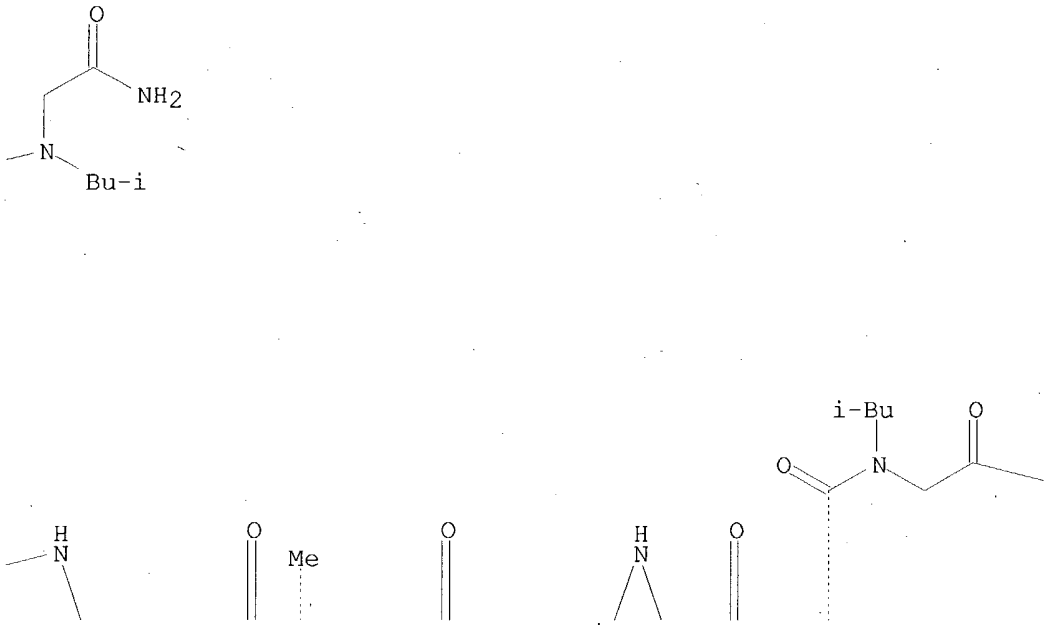

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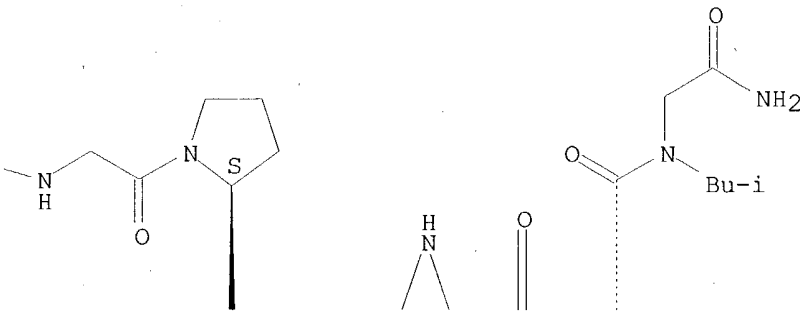

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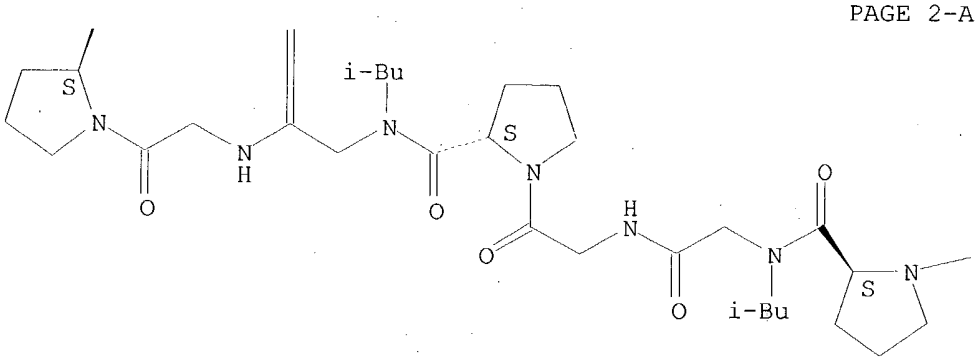

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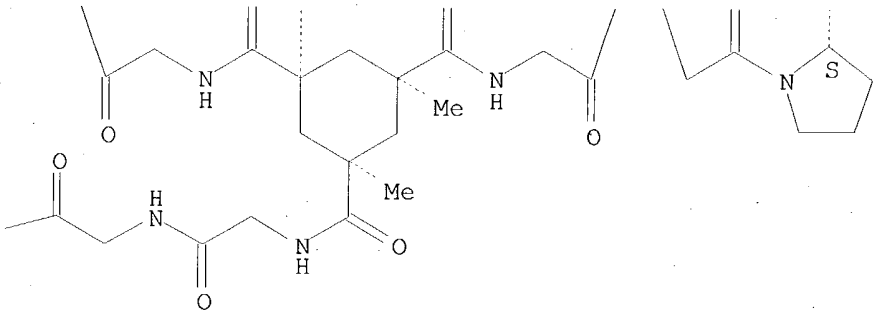

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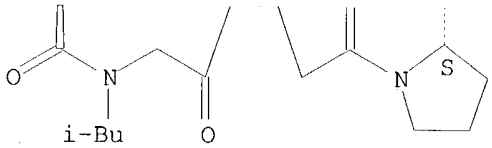
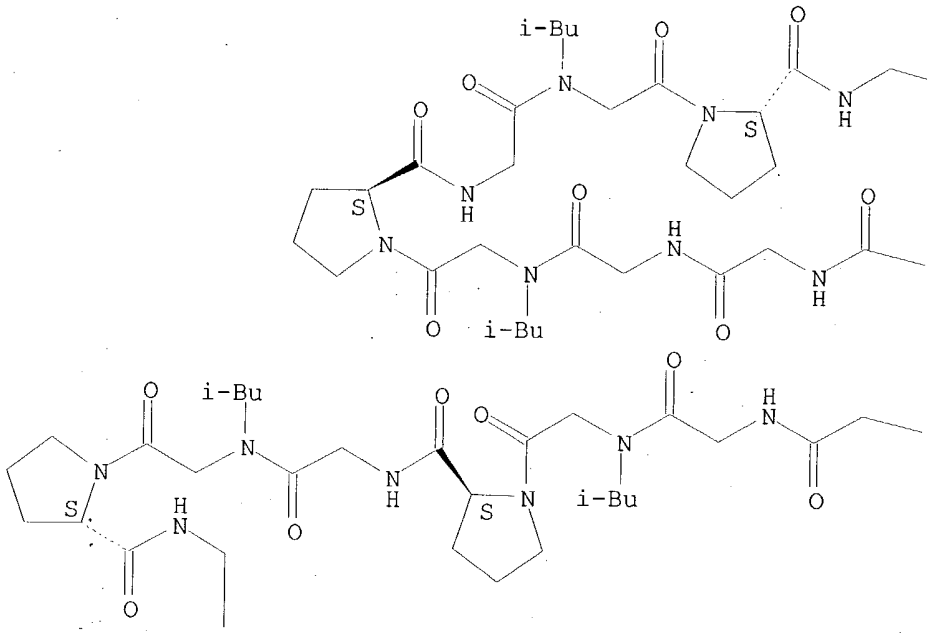


RN 191537-50-5 HCAPLUS
CN L-Prolinamide, 1,1',1''-[[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-trimethyl-1,3,5-cyclohexanetriyl]tricarbonyl]tris[glycylglycyl-N-(2-methylpropyl)glycyl-L-prolylglycyl-N-(2-methylpropyl)glycyl-L-prolylglycyl-N-(2-methylpropyl)glycyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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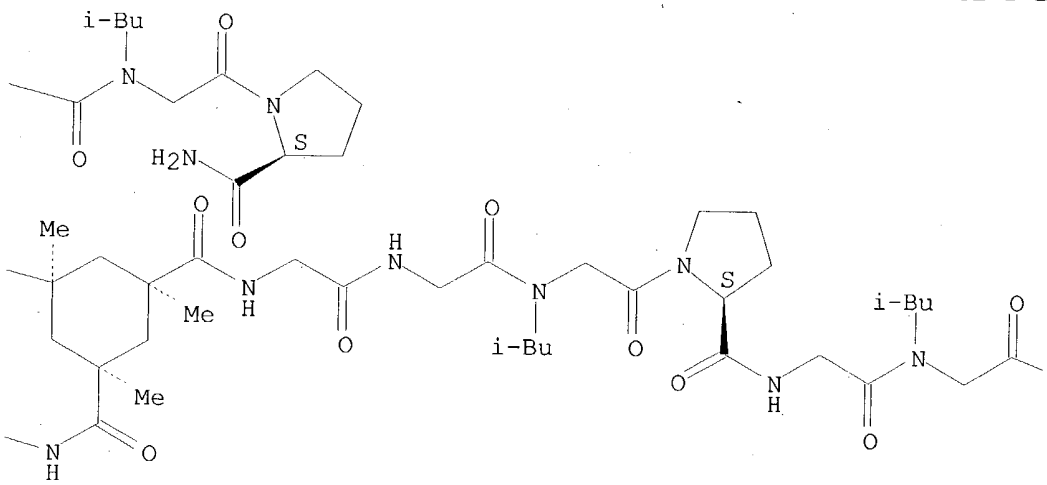

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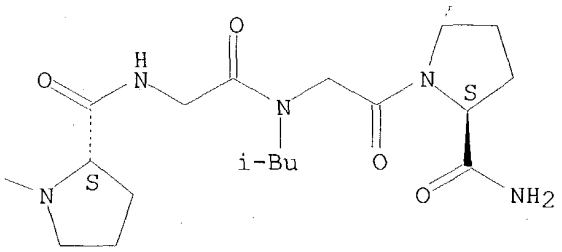

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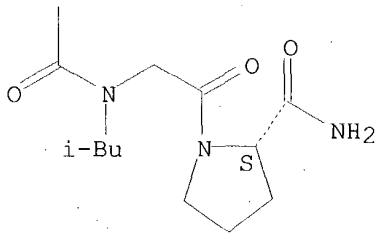


L27 ANSWER 36 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1997:425133 HCAPLUS
DOCUMENT NUMBER: 127:77487
TITLE: Collagen-Based Structures Containing the Peptoid Residue N-Isobutylglycine (Nleu): Conformational Analysis of Gly-Nleu-Pro Sequences by 1H-NMR and Molecular Modeling
AUTHOR(S): Melacini, Giuseppe; Feng, Yangbo; Goodman, Murray
CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of California at San Diego, La Jolla, CA, 92093-0343, USA
SOURCE: Biochemistry (1997), 36(29), 8725-8732
CODEN: BICHAW; ISSN: 0006-2960
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Mol. modeling and 1H-NMR were employed to study the structure and stability of collagen-like triple helixes composed of Gly-Nleu-Pro repeats. The compds. studied include the acetyl analogs Ac-(Gly-Nleu-Pro)n-NH2 (where n = 1, 3, 6, and 10) and the KTA conjugates KTA-[Gly-(Gly-Nleu-Pro)n-NH2]3 (where n = 3 and 6 and KTA denotes the Kemp triacid). The presence of collagen-like assembled structures is supported by a consistent set of exptl. observations, which include the appearance of a distinct set of resonances, low hydrogen-exchange rates for Gly NH, cooperative melting transition, and observation of several interchain NOEs. Using 1H-NMR, the triple helicity was monitored as a function of chain length, template, and temp. These studies show that (Gly-Nleu-Pro)n sequences have a somewhat higher triple-helical propensity than

(Gly-Pro-Nleu)n sequences. In addn., our investigations have shown that unlike the triple helixes composed of Gly-Pro-Nleu repeats those composed of Gly-Nleu-Pro repeats can access conformations in which the Nleu side chains are arrayed between Pro residues belonging to different triple-helix cross sections. These structural features may serve as a basis for free energy computations and for the study of higher-order structures such as collagen-like fibrils contg. peptoid moieties.

IT **191537-50-5**

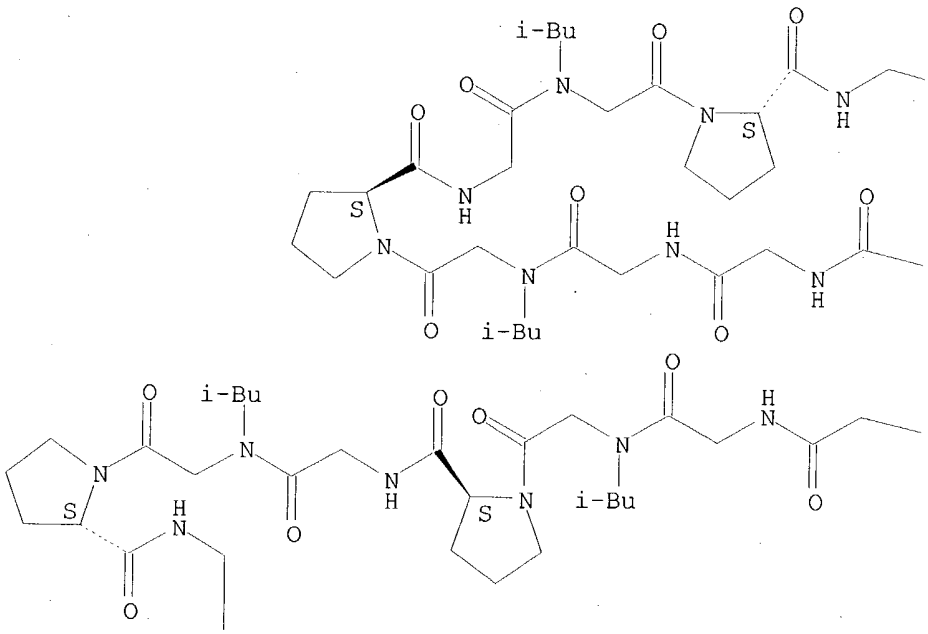
RL: PRP (Properties)
(conformational anal. of collagen-based Gly-Nleu-Pro sequences contg. the peptoid residue N-isobutylglycine (Nleu) by 1H-NMR and mol. modeling)

RN 191537-50-5 HCAPLUS

CN L-Prolinamide, 1,1',1''-[[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-trimethyl-1,3,5-cyclohexanetriyl]tricarbonyl]tris[glycylglycyl-N-(2-methylpropyl)glycyl-L-prolylglycyl-N-(2-methylpropyl)glycyl-L-prolylglycyl-N-(2-methylpropyl)glycyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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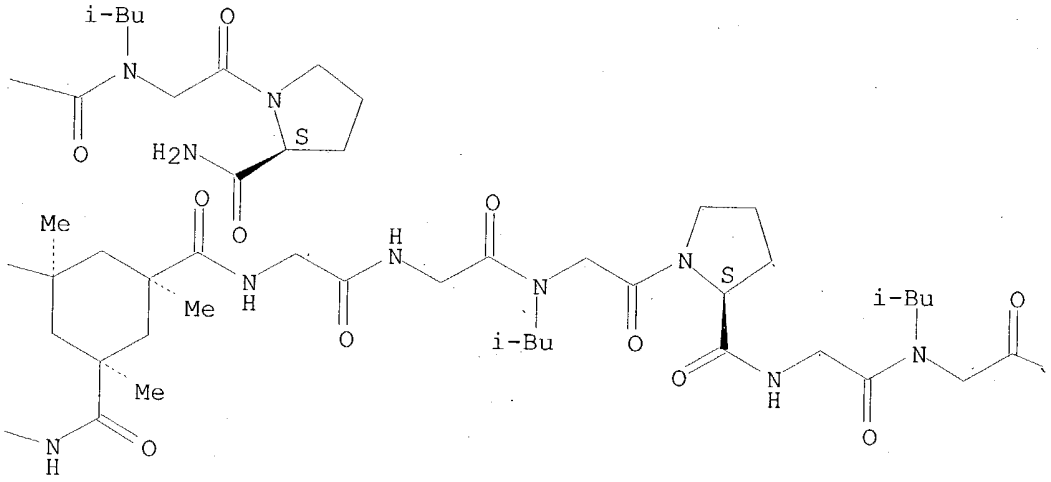

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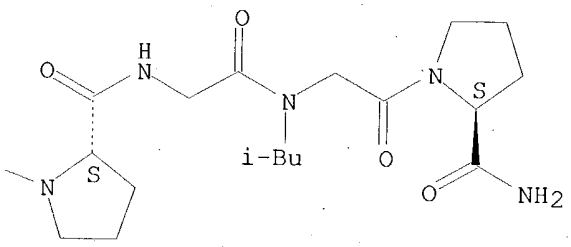

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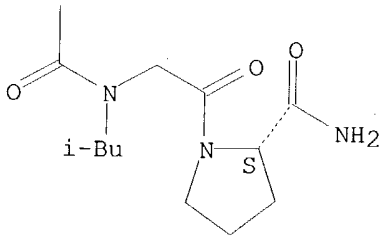


L27 ANSWER 37 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1997:425132 HCAPLUS
DOCUMENT NUMBER: 127:77486
TITLE: Collagen-Based Structures Containing the Peptoid Residue N-Isobutylglycine (Nleu): Synthesis and

Biophysical Studies of Gly-Nleu-Pro Sequences by Circular Dichroism and Optical Rotation

AUTHOR(S): Feng, Yangbo; Melacini, Giuseppe; Goodman, Murray
CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of California at San Diego, La Jolla, CA, 92093-0343, USA

SOURCE: Biochemistry (1997), 36(29), 8716-8724
CODEN: BICHAW; ISSN: 0006-2960
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

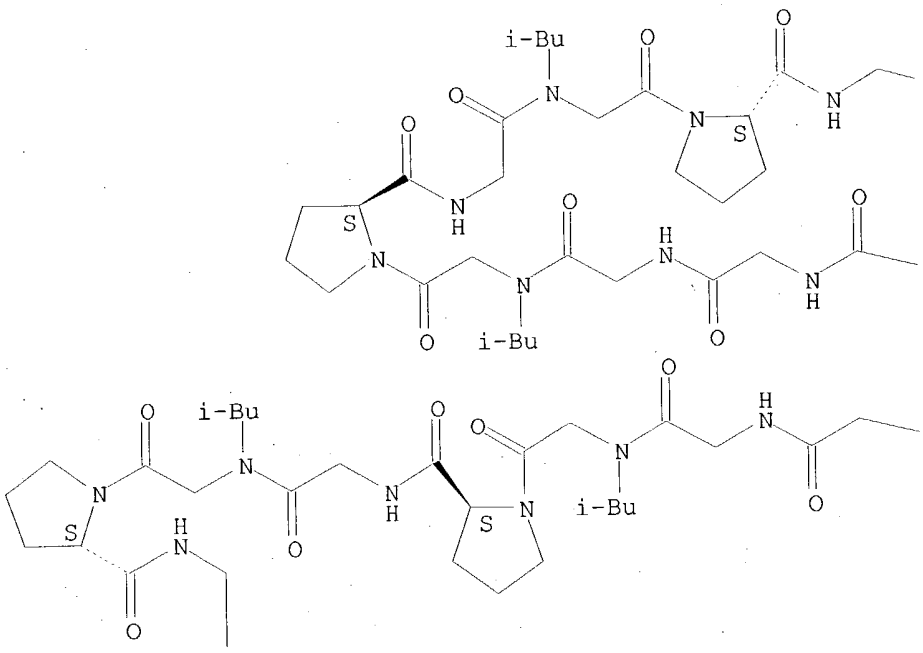
AB Single-chain peptide-peptoid structures, Ac-(Gly-Nleu-Pro)n-NH2 (n = 3, 6, and 10) and (Gly-Nleu-Pro)n-NH2 (n = 1 and 9), and template-assembled collagen analogs, KTA-[Gly-(Gly-Nleu-Pro)n-NH2]3 (n = 3 and 6; KTA represents cis,cis-1,3,5-trimethylcyclohexane-1,3,5-tricarboxylic acid, also known as the Kemp triacid; Nleu denotes N-isobutylglycine), were prepd. by solid-phase peptide synthesis methods. Biophys. studies using CD and optical rotation measurements show that these collagen analogs form triple-helical conformations when the chain is longer than a crit. length. Unlike collagen-based structures composed of Gly-Pro-Hyp and Gly-Pro-Nleu sequences, results reveal that the presence of a pos. CD peak between 220 and 225 nm is indicative of triple-helical conformations for these collagen-based structures composed of Gly-Nleu-Pro sequences. Results also indicate that the Gly-Nleu-Pro sequence possesses a higher triple-helical propensity than the Gly-Pro-Nleu sequence as demonstrated by the higher melting temps., the faster triple-helix folding, and the lower min. concn. necessary to detect triple-helicity for the single-chain structures. Therefore, we conclude that the Nleu residue in the second position of the trimeric repeat is more effective in inducing triple-helix formation than Pro in the same position.

IT **191537-50-5P**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(synthesis and triple-helical propensities of collagen-based structures contg. the peptoid residue N-isobutylglycine (Nleu) in Gly-Nleu-Pro sequences)

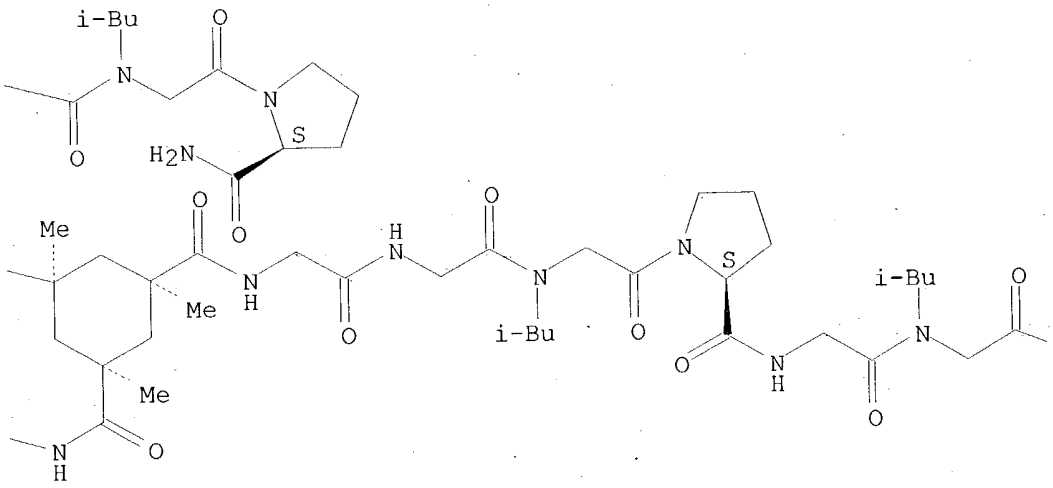
RN 191537-50-5 HCAPLUS
CN L-Prolinamide, 1,1',1''-[[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-trimethyl-1,3,5-cyclohexanetriyl]tricarbonyl]tris[glycylglycyl-N-(2-methylpropyl)glycyl-L-prolylglycyl-N-(2-methylpropyl)glycyl-L-prolylglycyl-N-(2-methylpropyl)glycyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



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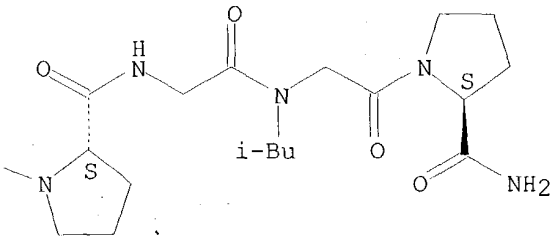

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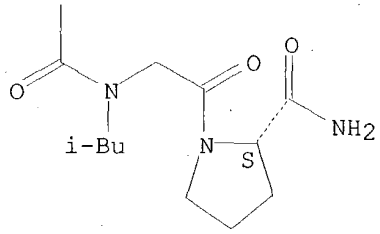


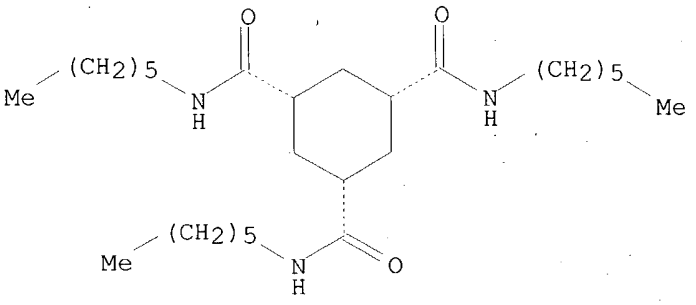
L27 ANSWER 38 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1997:175440 HCAPLUS
DOCUMENT NUMBER: 126:309200
TITLE: Small molecular gelling agents to harden organic liquids: trialkyl cis-1,3,5-cyclohexanetricarboxamides
AUTHOR(S): Hanabusa, Kenji; Kawakami, Atsushi; Kimura, Mutsumi; Shirai, Hirofusa
CORPORATE SOURCE: Faculty of Textile Science & Technology, Shinshu University, Ueda, 386, Japan
SOURCE: Chemistry Letters (1997), (3), 191-192
CODEN: CMLTAG; ISSN: 0366-7022
PUBLISHER: Nippon Kagakkai
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Trialkyl cis-1,3,5-cyclohexanetricarboxamides were able to cause phys. gelation in org. liqs. to afford completely transparent organogel. The main driving force for gelation was intermol. hydrogen bonding between amides and van der Waals interaction among hydrophobic alkyl chains.

IT **189299-28-3 189299-29-4 189299-30-7 189301-40-4**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(phys. gelation of trialkyl cis-1,3,5-cyclohexanetricarboxamides in org. liqs.)

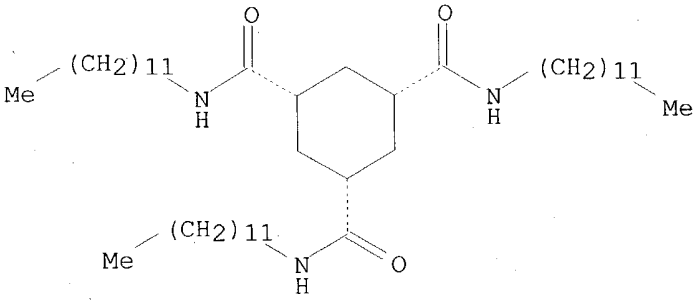
RN 189299-28-3 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-trihexyl-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



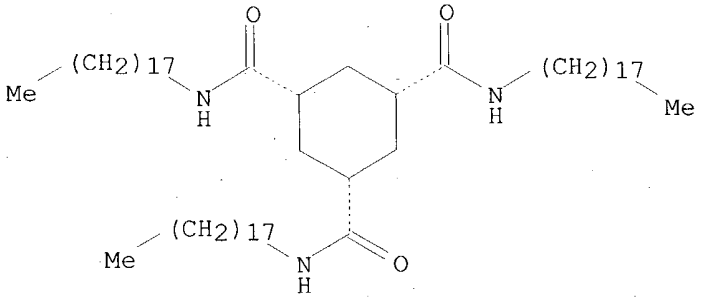
RN 189299-29-4 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tridodecyl-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 189299-30-7 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-trioctadecyl-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

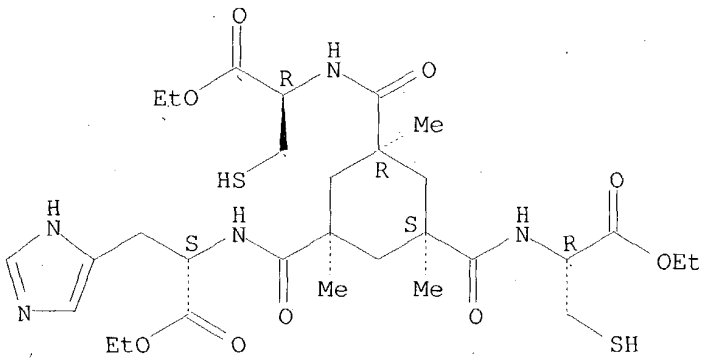
Relative stereochemistry.



RN 189301-40-4 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris(3,7-dimethyloctyl)-, (1.alpha.,3.alpha.,5.alpha.)-[partial]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Absolute stereochemistry.



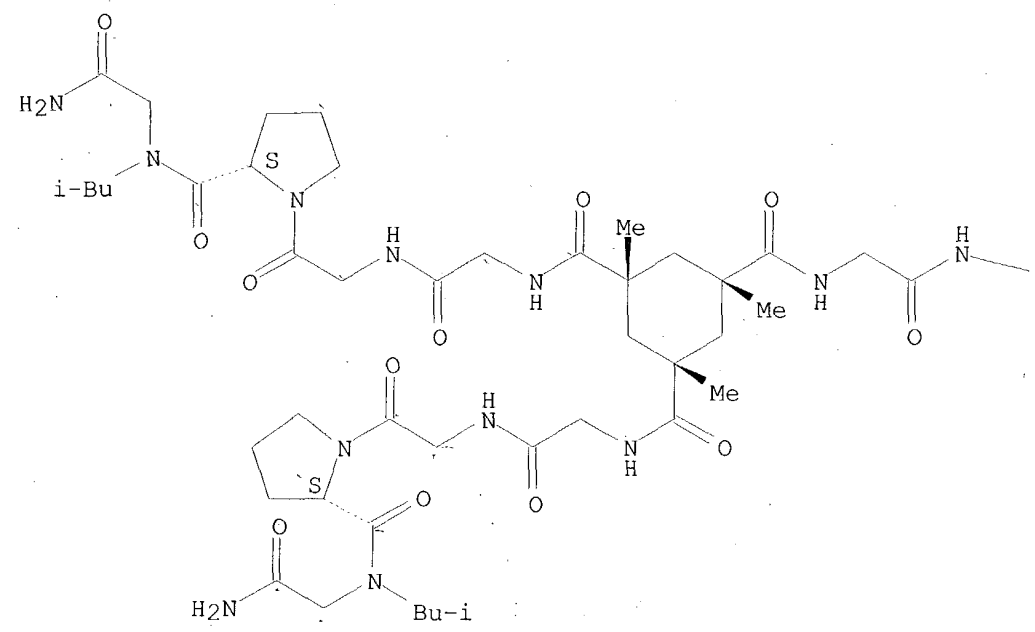
L27 ANSWER 40 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1996:750209 HCAPLUS
DOCUMENT NUMBER: 126:118179
TITLE: Collagen-based structures containing the peptoid residue N-isobutylglycine (NLeu): Synthesis and biophysical studies of Gly-Pro-NLeu sequences by circular dichroism, ultraviolet absorbance, and optical rotation
AUTHOR(S): Feng, Yangbo; Melacini, Giuseppe; Taulane, Joseph P.; Goodman, Murray
CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of California San Diego, La Jolla, CA, 92093-0343, USA
SOURCE: Biopolymers (1996), 39(6), 859-872
CODEN: BIPMAA; ISSN: 0006-3525
PUBLISHER: Wiley
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A peptoid residue N-isobutylglycine (NLeu) was introduced as a proline surrogate in collagen-like triple helical structures. A series of single chain and template-assembled collagen-based peptide-peptoid structures composed of Gly-Pro-NLeu sequences were prepd. by solid phase segment condensation methods. Both a synthetic route in soln. and a solid phase method were employed to couple the KTA (cis,cis-1,3,5-trimethylcyclohexane-1,3,5-tricarboxylic acid, also known as the Kemp triacid) based template, KTA-(Gly-OH)3 to peptide-peptoid chains. Biophys. studies using CD, UV, and optical rotation measurements demonstrated that these compds. form triple-helical structures when the chains are longer than crit. lengths. Results from melting curve measurements indicated that the Gly-Pro-NLeu sequence is comparable to the Gly-Pro-Pro sequence in stabilizing a triple-helical conformation. The KTA-based template stabilized triple-helical structures as can be seen by the increased melting temps. as compared to equiv. single chain mols. In addn., the template reduced the min. chain length necessary to form a triple helix from six to only three trimer repeats.

IT **186031-88-9P 186031-89-0P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and biophys. properties of collagen-based structures contg. isobutylglycine peptoid residues)
RN 186031-88-9 HCAPLUS
CN Glycinamide, 1,1',1''-[[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-trimethyl-1,3,5-cyclohexanetriyl]tricarbonyl]tris[glycylglycyl-L-prolyl-N2-(2-methylpropyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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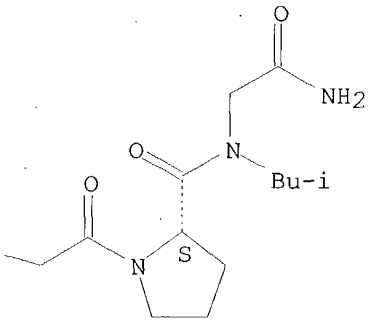
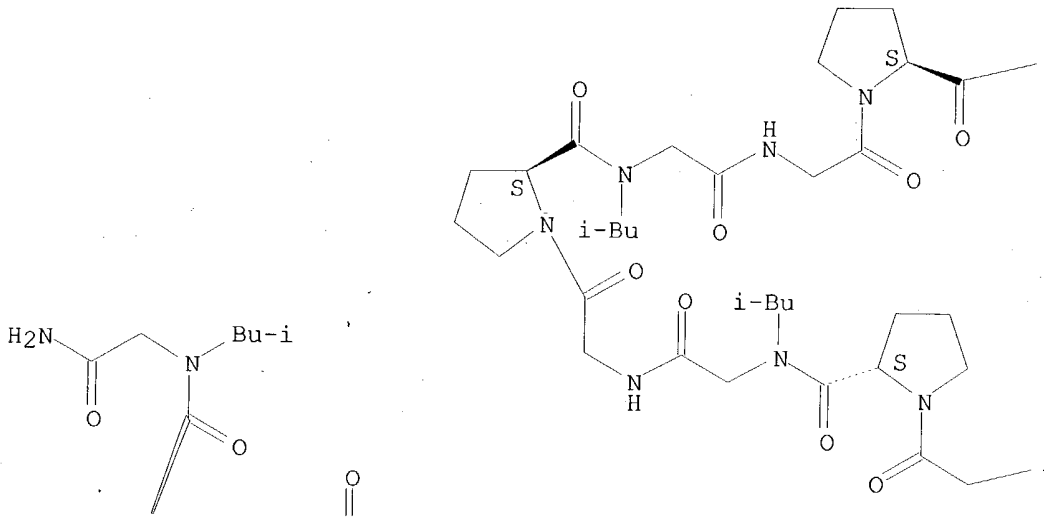


RN 186031-89-0 HCAPLUS
CN Glycinamide, 1,1',1''-[[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-trimethyl-1,3,5-cyclohexanetriyl]tricarbonyl]tris[glycylglycyl-L-prolyl-N-(2-methylpropyl)glycylglycyl-L-prolyl-N-(2-methylpropyl)glycylglycyl-L-prolyl-N2-(2-methylpropyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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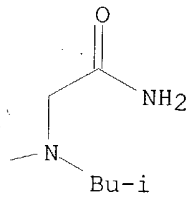

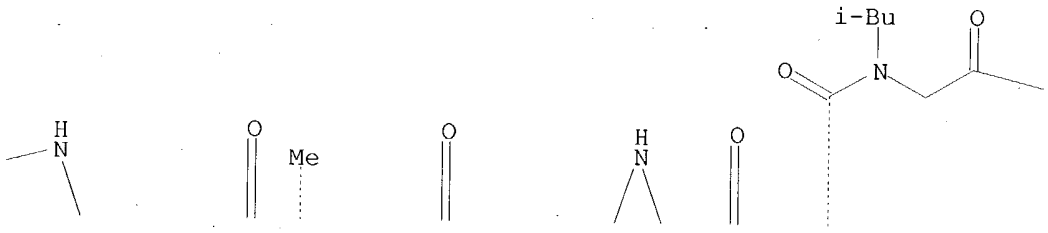

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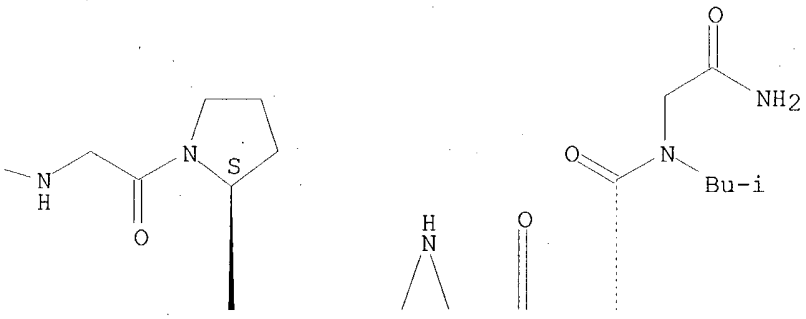
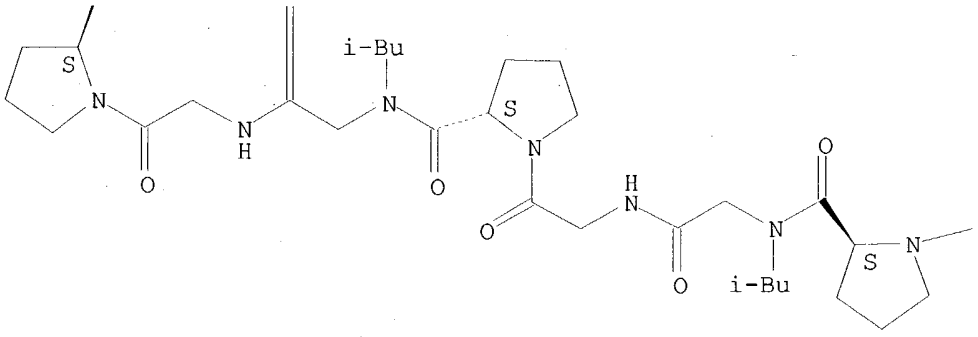


PAGE 2-A



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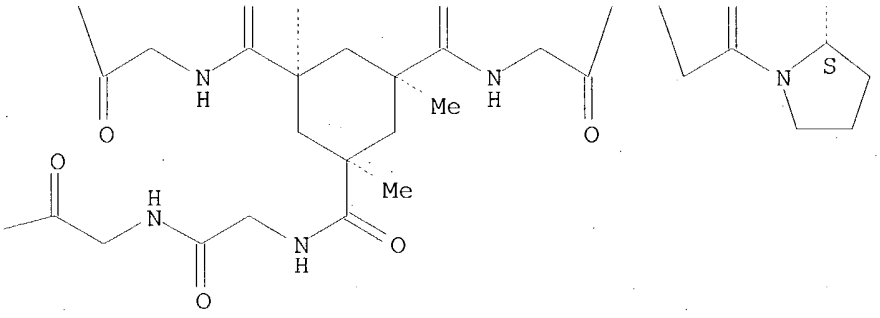

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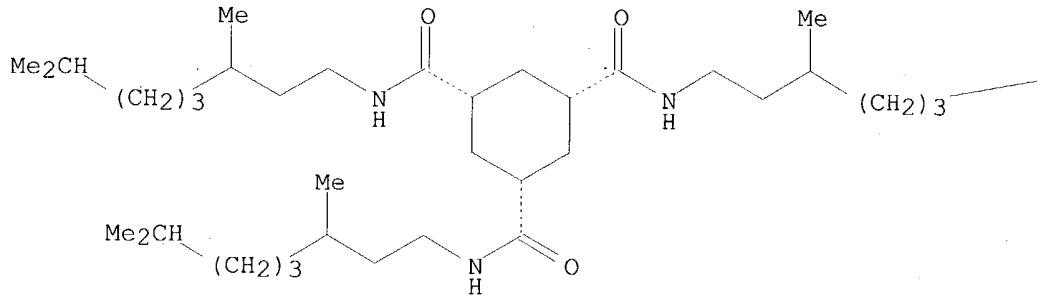

PAGE 1-B

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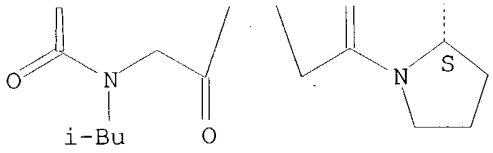
REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 39 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1997:143376 HCAPLUS
DOCUMENT NUMBER: 126:222195
TITLE: Model molecules for the active center of alcohol dehydrogenases-An FT-IR study
AUTHOR(S): Brzezinski, Bogumil; Urjasz, Hanna; Zundel, Georg; Bartl, Franz
CORPORATE SOURCE: Faculty of Chemistry, Adam Mickiewicz University, Poznan, 60 780, Pol.
SOURCE: Biochemical and Biophysical Research Communications (1997), 231(2), 473-476
CODEN: BBRCA9; ISSN: 0006-291X
PUBLISHER: Academic
DOCUMENT TYPE: Journal
LANGUAGE: English

AB We synthesized a triamide of Kemp's acid with two cysteine groups and one histidine group (compd. 1), and a triamide of 1,3,5-pentane tricarboxylic acid with tyrosine, histidine, and arginine mols. (compd. 2). From compd. 1 we obtained the hydrated Zn2+ complex, compd. 3. The FT-IR spectra of various complexes of compds. 1-3 with NAD+ show no IR continua and hence, no hydrogen-bonded chains with proton polarizability are present. In the case of the complex (compds. 2 and 3 and NAD+) an intense continuum demonstrates that a hydrogen-bonded chain is formed with large proton polarizability due to collective proton motion. This proton pathway is discussed. The O atom of the nicotinamide group of NAD+ is a strong hydrogen bond acceptor. This result is discussed with regard to the catalytic mechanism.

IT **188351-53-3P**
RL: BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(model mols. for the active center of alc. dehydrogenases-an FT-IR study)

RN 188351-53-3 HCAPLUS
CN L-Histidine, N-[[(1R,3R,5S)-3,5-bis[[[(1R)-2-ethoxy-1-(mercaptomethyl)-2-oxoethyl]amino]carbonyl]-1,3,5-trimethylcyclohexyl]carbonyl]-, ethyl ester (9CI) (CA INDEX NAME)



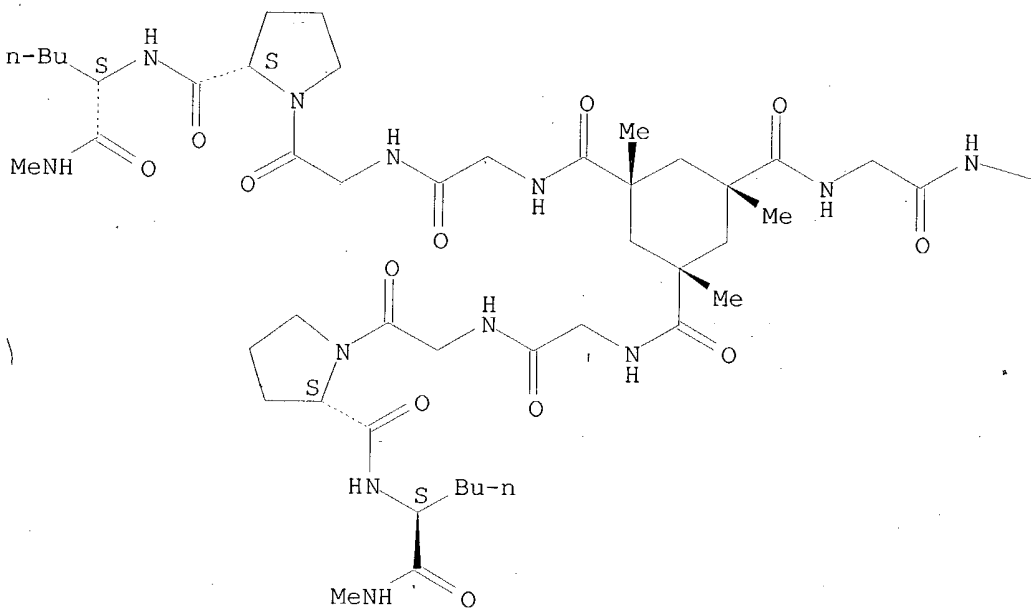
L27 ANSWER 41 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1996:625561 HCAPLUS
DOCUMENT NUMBER: 126:15960
TITLE: Collagen-Based Structures Containing the Peptoid Residue N-Isobutylglycine (Nleu): Conformational Analysis of Gly-Pro-Nleu Sequences by 1H NMR, CD, and Molecular Modeling
AUTHOR(S): Melacini, Giuseppe; Feng, Yangbo; Goodman, Murray
CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of California at San Diego, La Jolla, CA, 92093-0343, USA
SOURCE: Journal of the American Chemical Society (1996), 118(44), 10725-10732
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Mol. modeling, 1H NMR, and CD were employed to study the structure and stability of collagen-like triple helixes composed of Gly-Pro-Nleu repeats. The compds. studied include the acetyl analogs Ac-(Gly-Pro-Nleu)n-NH2 (where n = 1, 6, 9) and the KTA conjugates KTA-[Gly-(Gly-Pro-Nleu)n-NH2]3 (where n = 1, 3, 6, 9 and KTA denotes the Kemp triacid). The presence of collagen-like assembled structures was supported by a consistent set of exptl. observations, including the appearance of a distinct set of resonances, low hydrogen exchange rates for Gly NH, KTA signal splitting, cooperative melting transition, and anal. of NOESY cross peaks. In this regard, the concept of ensemble interchain NOEs was introduced and used to establish the close packing of Gly, Pro, and Nleu residues in triple helixes composed of Gly-Pro-Nleu repeats. In addn., the ensemble interchain NOEs gave insight into the puckering of the Pro ring and the conformations accessible to the Nleu side chain. The effect of the KTA template on triple helicity was studied and shown to consist in a net gain in the free energy of triple-helix formation, as also seen for Gly-Pro-Hyp sequences. This free energy gain led to the induction of an assembled collagen-like structure in the KTA conjugate contg. six Gly-Pro-Nleu repeats per chain and to an increase in thermal stability of the compd. contg. nine Gly-Pro-Nleu repeats per chain.

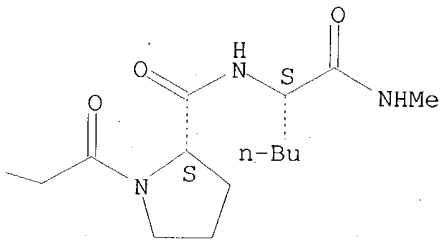
IT **184017-05-8 184017-06-9**
RL: PRP (Properties)
(conformational anal. of collagen-like triple helixes composed of Gly-Pro-Nleu repeats)
RN 184017-05-8 HCAPLUS
CN L-Norleucinamide, 1,1',1''-[[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-trimethyl-1,3,5-cyclohexanetriyl]tricarbonyl]tris[glycylglycyl-L-prolyl-N-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



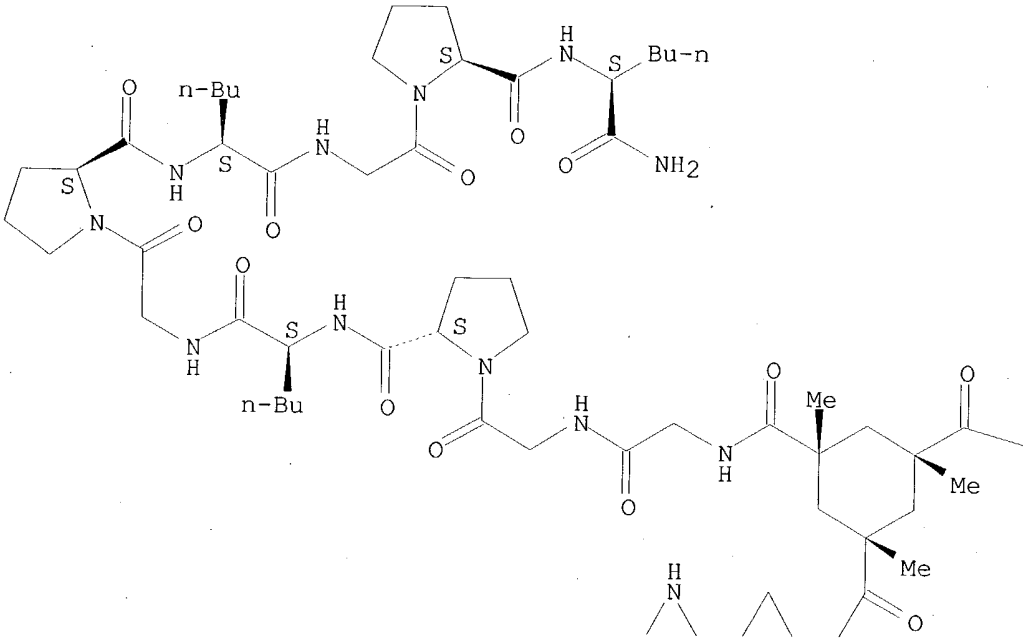
PAGE 1-B



RN 184017-06-9 HCAPLUS
CN L-Norleucinamide, 1,1',1''-[[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-trimethyl-1,3,5-cyclohexanetriyl]tricarbonyl]tris[glycylglycyl-L-prolyl-L-norleucylglycyl-L-prolyl-L-norleucylglycyl-L-prolyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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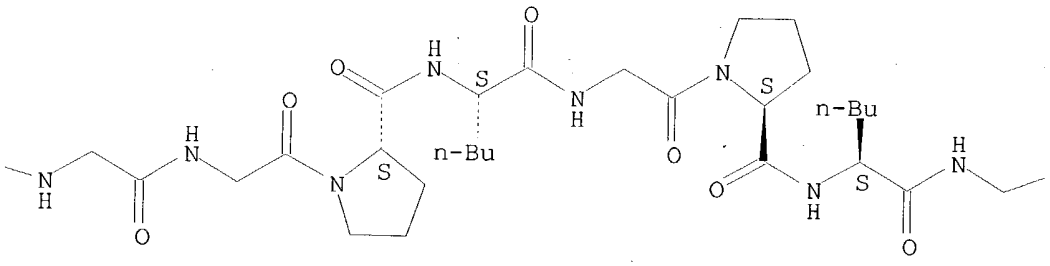

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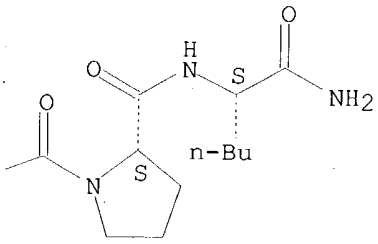

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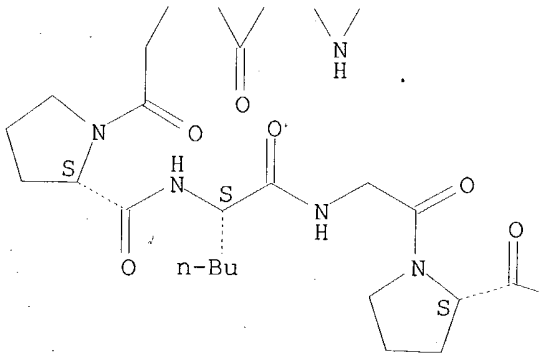
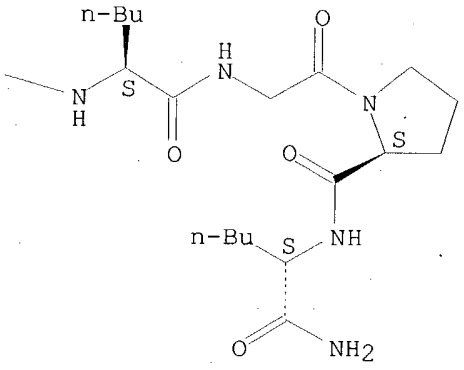




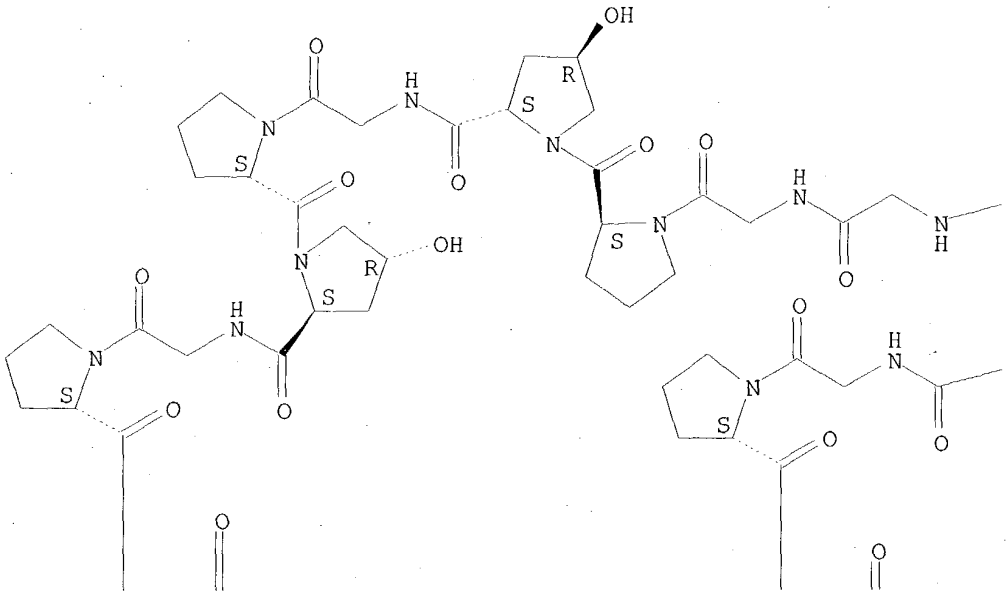
L27 ANSWER 42 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1996:616678 HCAPLUS
DOCUMENT NUMBER: 126:75222
TITLE: Acetyl-Terminated and Template-Assembled Collagen-Based Polypeptides Composed of Gly-Pro-Hyp Sequences. 2. Conformational Analysis by 1H-NMR and Molecular Modeling Studies
AUTHOR(S): Melacini, Giuseppe; Feng, Yangbo; Goodman, Murray
CORPORATE SOURCE: Department of Chemistry Biochemistry, University of California, La Jolla, CA, 92093-0343, USA
SOURCE: Journal of the American Chemical Society (1996), 118(43), 10359-10364
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Using 1- and 2-dimensional 1H-NMR and mol. modeling, the conformational features of template-assembled collagen-like polypeptides of the type KTA-[Gly-(Gly-Pro-Hyp)n-NH2]3 (I; n = 1, 3, 5, 6; KTA = Kemp's triacid) and of the corresponding acetylated single-chain polypeptides Ac-(Gly-Pro-Hyp)n-NH2 (n = 1, 3, 5, 6, 9) were characterized in water. The presence of triple-helical conformations was established on the basis of consistent exptl. observations including the appearance of a set of distinct assembled resonances and the measurement of low hydrogen-exchange rates for the assembled Gly NH of the longer chain analogs. In addn., following the pioneering work of M.-H. Li, P. Fan, B. Brodsky, and J. Baum (1993), the consistency of the NOESY spectra with the interchain NOEs anticipated by the X-ray model for triple-helical (Gly-Pro-Hyp) sequences was proved. For I, the triple helicity is further supported by the KTA signal splitting detected for I (n = 3, 5, 6) and caused by the triple-helical screw symmetry which breaks the rotational symmetry of KTA. Thermal melting studies indicate that the KTA template leads to a significant gain in the free energy of triple-helix formation. This free energy gain results in a remarkable increase of the thermal stabilities of the KTA terminated compds. as compared to the acetyl analogs. The NMR results are fully consistent with the author's previous investigations based on CD, UV, and optical rotation spectroscopic methods.

IT **176839-96-6 183888-57-5**
RL: PRP (Properties)
(conformational anal. of acetyl-terminated and template-assembled collagen-based polytripeptides by NMR and mol. modeling)
RN 176839-96-6 HCAPLUS
CN L-Prolinamide, 1,1',1''-[[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-trimethyl-1,3,5-cyclohexanetriyl]tricarbonyl]tris[glycylglycyl-L-prolyl-(4R)-4-hydroxy-L-prolylglycyl-L-prolyl-(4R)-4-hydroxy-L-prolylglycyl-L-prolyl-4-hydroxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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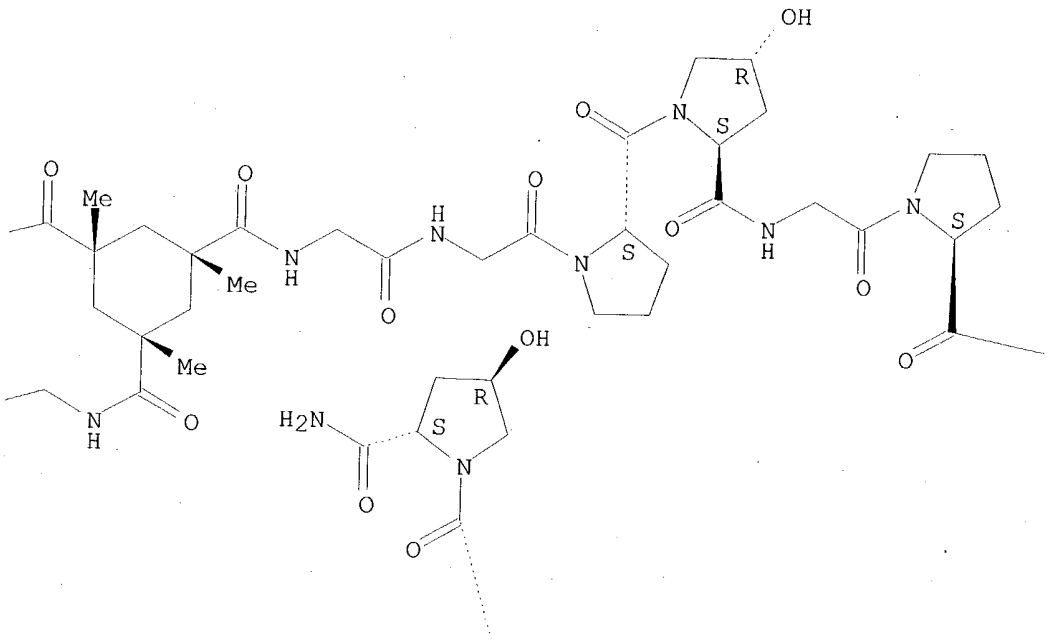

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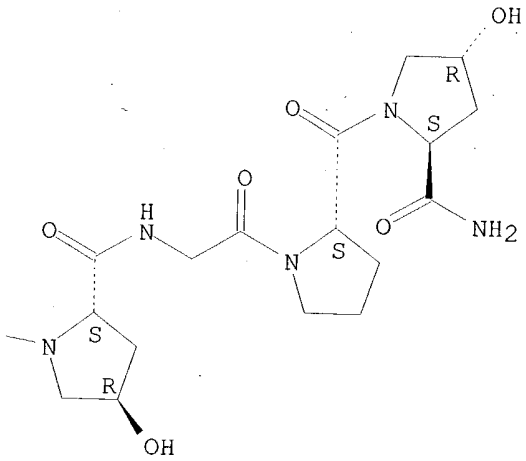
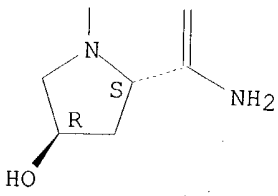
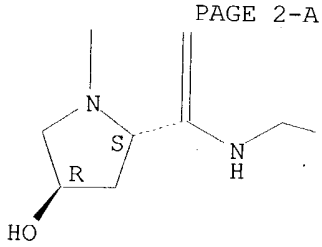
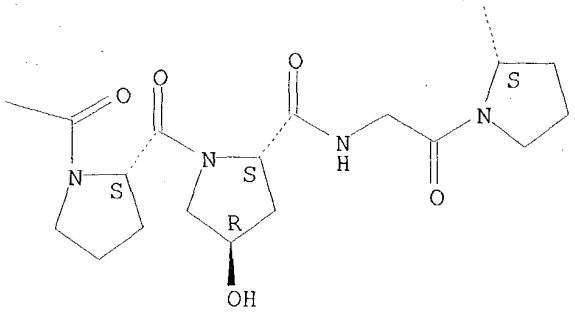




PAGE 2-A



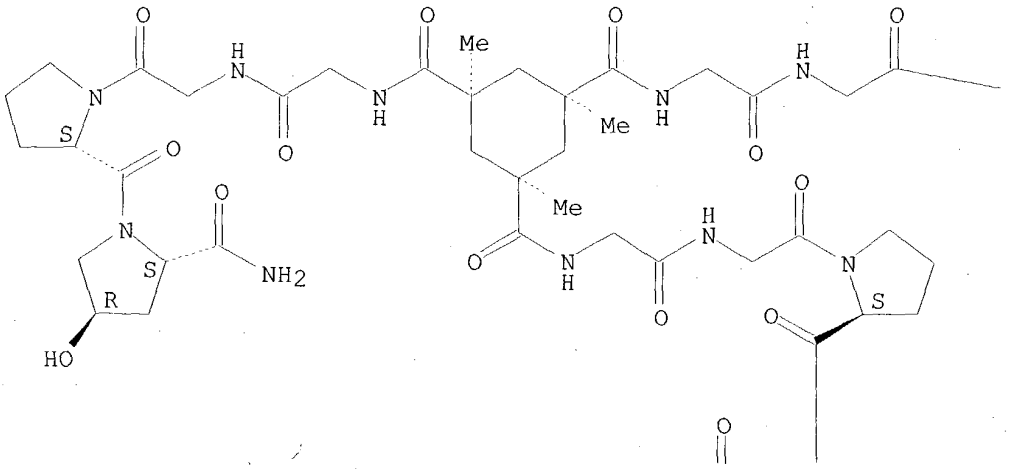
PAGE 2-B



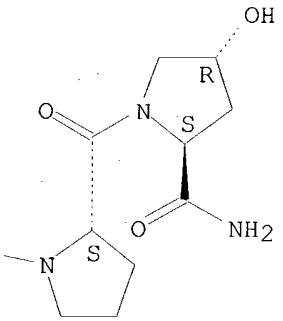
RN 183888-57-5 HCAPLUS
CN L-Prolinamide, 1,1',1''-[[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-trimethyl-1,3,5-cyclohexanetriyl]tricarbonyl]tris[glycylglycyl-L-prolyl-4-hydroxy-, (4R,4'R,4''R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

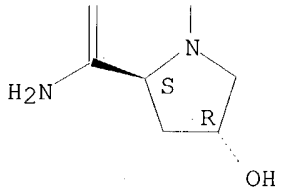
PAGE 1-A



PAGE 1-B



PAGE 2-A



L27 ANSWER 43 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1996:616677 HCAPLUS
DOCUMENT NUMBER: 126:75221
TITLE: Acetyl-Terminated and Template-Assembled Collagen-Based Polypeptides Composed of Gly-Pro-Hyp Sequences. 1. Synthesis and Conformational Analysis by Circular Dichroism, Ultraviolet Absorbance, and Optical Rotation
AUTHOR(S): Feng, Yangbo; Melacini, Giuseppe; Taulane, Joseph P.; Goodman, Murray
CORPORATE SOURCE: Department of Chemistry Biochemistry, University of California at San Diego, La Jolla, CA, 92093-0343, USA
SOURCE: Journal of the American Chemical Society (1996), 118(43), 10351-10358
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Template-assembled collagen-based polypeptides KTA-[Gly-(Gly-Pro-Hyp)n-NH2]3 [I; n = 1, 3, 5, 6; KTA = cis,cis-1,3,5-trimethylcyclohexane-1,3,5-tricarboxylic acid (Kemp's triacid)] and acetyl-terminated single-chain collagen-based analogs Ac-(Gly-Pro-Hyp)n-NH2 (II; n = 1, 3, 5, 6, 9) were synthesized by solid phase segment condensation methods. The triple-helical propensities of these collagen analogs were investigated using CD, UV absorbance, optical rotation, and NMR measurements. The acetyl analogs, II (n = 6, 9), assume a stable triple-helical conformation in H2O (0.2 mg/mL) at room temp. By contrast, II (n = 5) adopts a triple-helical conformation in H2O only below 18.degree. at a concn. of 0.2 mg/mL. For the template-assembled collagen analogs, results show that I (n = 5, 6) peptides form triple-helical structures which have melting temps. above 70.degree. in H2O. These melting temps. are much higher than those of the corresponding acetyl analogs, demonstrating the significant triple-helix-stabilizing effects of the KTA template. In addn., the KTA template facilitates triple-helical structures by dramatically

accelerating triple-helix formation.

IT **176839-96-6P 183888-57-5P**

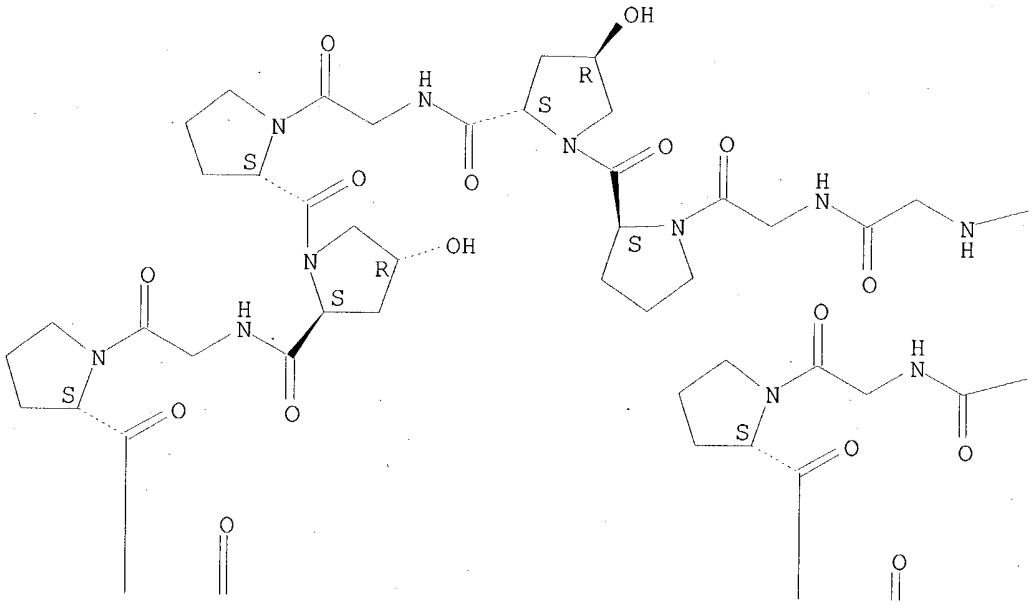
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (prepn. and conformational anal. of acetyl-terminated and template-assembled collagen-based polytripeptides)

RN 176839-96-6 HCAPLUS

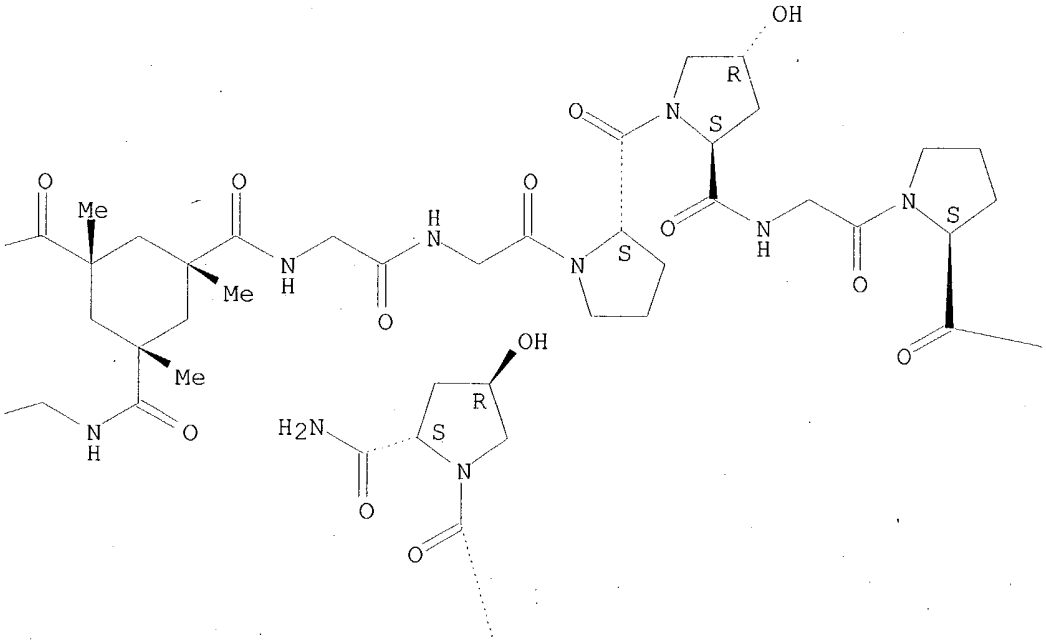
CN L-Prolinamide, 1,1',1''-[[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-trimethyl-1,3,5-cyclohexanetriyl]tricarbonyl]tris[glycylglycyl-L-prolyl-(4R)-4-hydroxy-L-prolylglycyl-L-prolyl-(4R)-4-hydroxy-L-prolylglycyl-L-prolyl-4-hydroxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

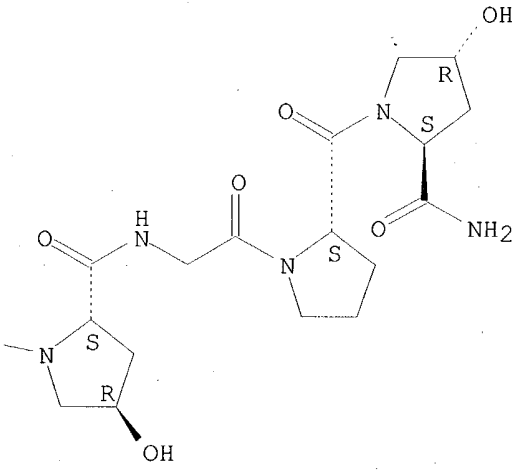
PAGE 1-A

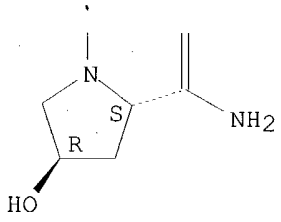


PAGE 1-B

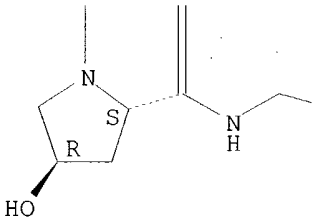


PAGE 1-C

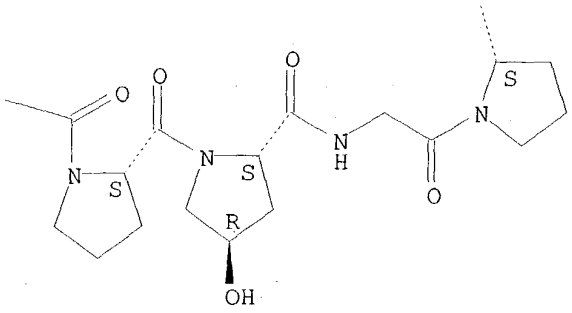




PAGE 2-A



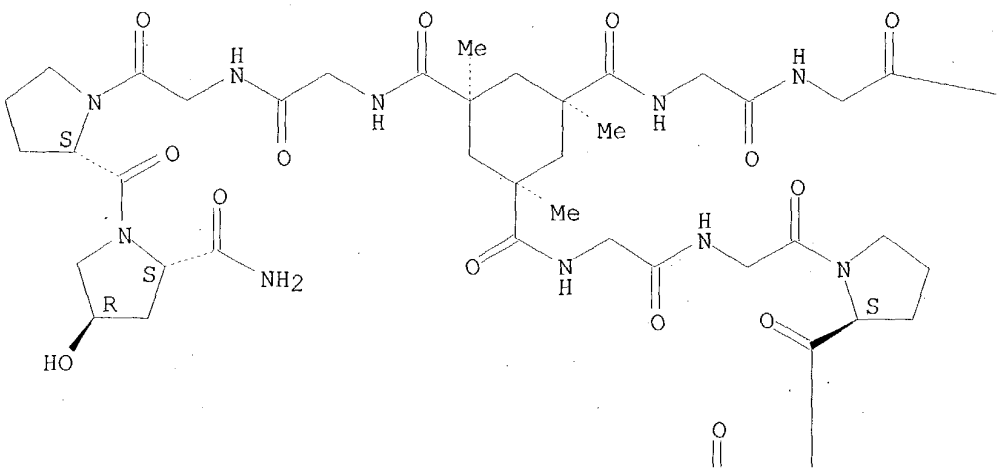
PAGE 2-B



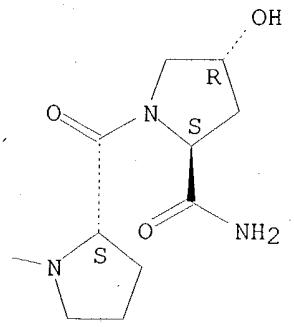
RN 183888-57-5 HCAPLUS
CN L-Prolinamide, 1,1',1''-[[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-trimethyl-1,3,5-cyclohexanetriyl]tricarbonyl]tris[glycylglycyl-L-prolyl-4-hydroxy-, (4R,4'R,4''R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

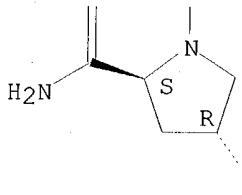
PAGE 1-A



PAGE 1-B



PAGE 2-A

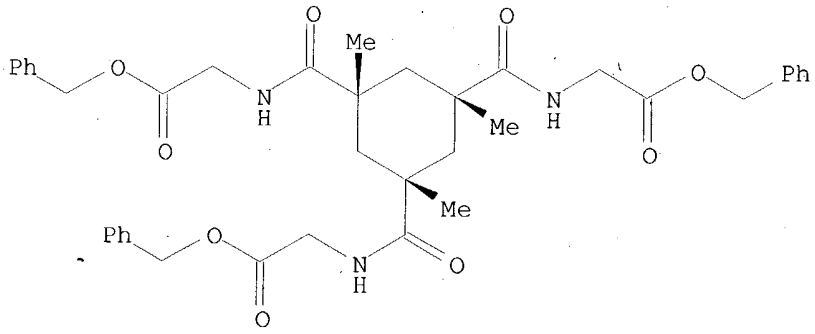


IT **183888-50-8P 183888-51-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and conformational anal. of acetyl-terminated and template-assembled collagen-based polytripeptides)

RN 183888-50-8 HCAPLUS

CN Glycine, N,N',N''-[[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-trimethyl-1,3,5-cyclohexanetriyl]tricarbonyl]tris-, tris(phenylmethyl) ester (9CI) (CA INDEX NAME)

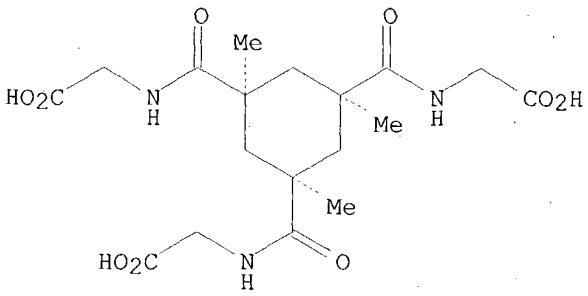
Relative stereochemistry.



RN 183888-51-9 HCAPLUS

CN Glycine, N,N',N''-[[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-trimethyl-1,3,5-cyclohexanetriyl]tricarbonyl]tris- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L27 ANSWER 44 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1996:567102 HCAPLUS
DOCUMENT NUMBER: 125:197514
TITLE: Crystalline resin compositions
INVENTOR(S): Ikeda, Naoki; Yoshimura, Masafumi; Mizoguchi, Kazuaki; Kitagawa, Hiroshi
PATENT ASSIGNEE(S): Shin Nippon Rika Kk, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

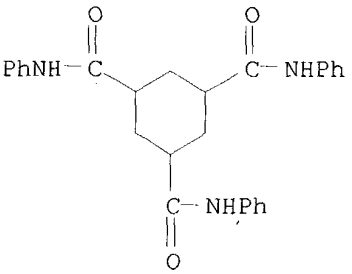
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 08157640	A2	19960618	JP 1995-170313	19950612

PRIORITY APPLN. INFO.: JP 1994-240112 19941004

AB Cryst. resins contain 0.001-10 phr .gtoreq.1 amide selected from amides of polycarboxylic acids, polyamines, and poly(amino acids) to improve crystn. rates. Thus, poly(phenylene sulfide) pellets contg. 0.2 phr terephthalic acid dicyclohexylamide had crystn. temp. 230.degree., compared with 191.degree. for the resin alone.

IT **160535-62-6**
RL: MOA (Modifier or additive use); USES (Uses)
(cryst. resin compns. contg. amides as nucleating agents)

RN 160535-62-6 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-triphenyl- (9CI) (CA INDEX NAME)



L27 ANSWER 45 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1996:285056 HCAPLUS
DOCUMENT NUMBER: 124:336180
TITLE: A Template-Induced Incipient Collagen-Like

Triple-Helical Structure

AUTHOR(S): Goodman, Murray; Feng, Yangbo; Melacini, Giuseppe; Taulane, Joseph P.

CORPORATE SOURCE: Department of Chemistry Biochemistry, University of California, San Diego, La Jolla, CA, 92093-0343, USA

SOURCE: Journal of the American Chemical Society (1996), 118(21), 5156-5157
CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A template-assembled polypeptide system that mimics the collagen-like triple helix is presented. A conformationally highly constrained org. structure, cis,cis-1,3,5-trimethylcyclohexane-1,3,5-tricarboxylic acid (also known as the Kemp triacid, KTA) was used as a template to nucleate the triple helical folding of three polypeptide chains, each of which contains only three glycyl-prolyl-hydroxyprolyl (Gly-Pro-Hyp) repeats. These three chains were linked to the KTA through glycine residues which act as spacers. The resulting system KTA-[Gly-(Gly-Pro-Hyp)3-NH2]3 assumes a triple helical conformation in H2O at room temp. as verified by 1H-NMR and optical rotation. Our results indicate that the short helical structure adopted by KTA-[Gly-(Gly-Pro-Hyp)3-NH2]3 exhibits some cooperativity and is significantly affected by triple helix and effects. We therefore define this assembled conformation as an incipient triple helix. To the best of our knowledge, this system represents the shortest chain collagen-like triple helical mol. which has been reported in the literature.

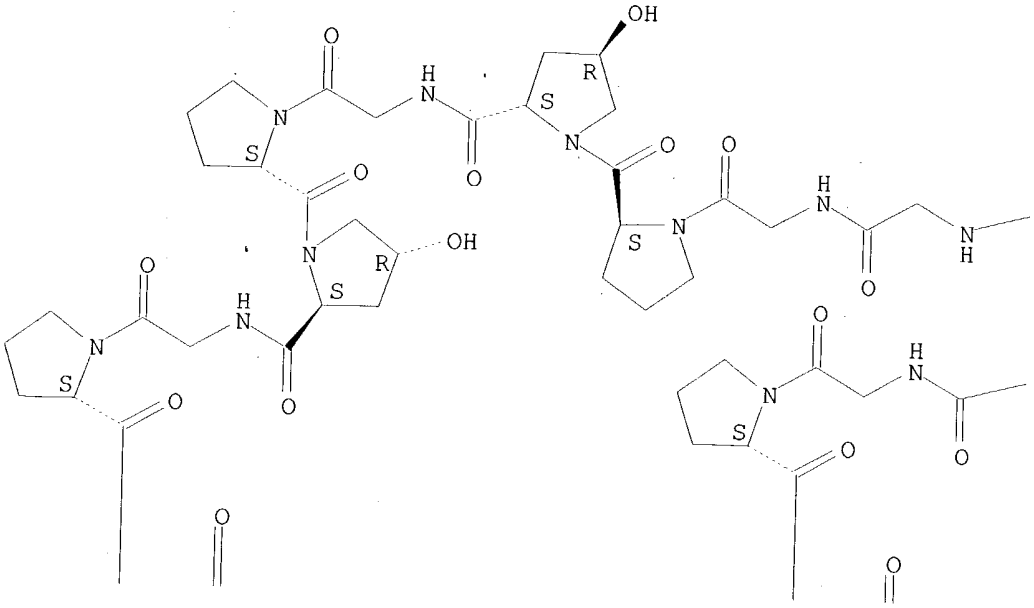
IT **176839-96-6P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(a template-induced incipient collagen-like triple-helical structure, KTA-[Gly-(Gly-Pro-Hyp)3-NH2]3)

RN 176839-96-6 HCAPLUS

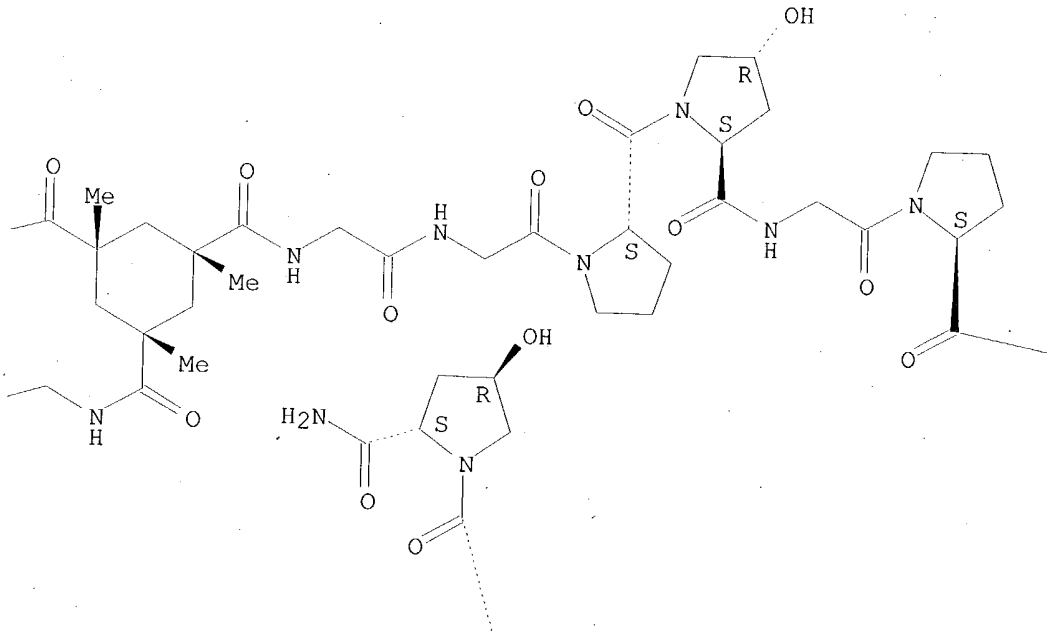
CN L-Prolinamide, 1,1',1''-[[(1.alpha.,3.alpha.,5.alpha.)-1,3,5-trimethyl-1,3,5-cyclohexanetriyl]tricarbonyl]tris[glycylglycyl-L-prolyl-(4R)-4-hydroxy-L-prolylglycyl-L-prolyl-(4R)-4-hydroxy-L-prolylglycyl-L-prolyl-4-hydroxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

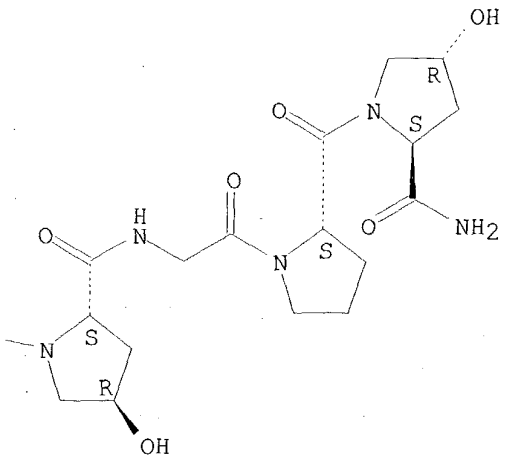
PAGE 1-A



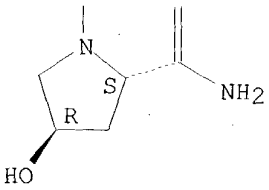
PAGE 1-B

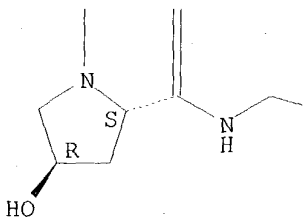


PAGE 1-C

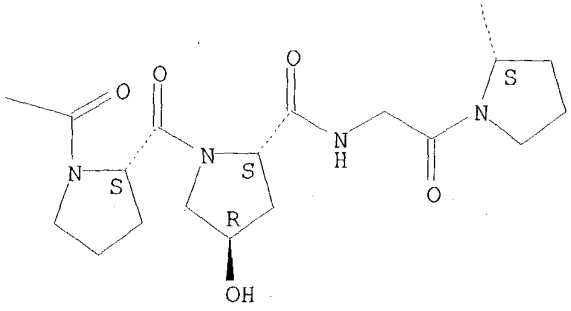


PAGE 2-A





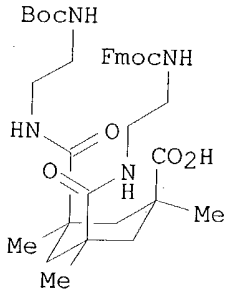
PAGE 2-B



L27 ANSWER 46 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1995:825831 HCAPLUS
DOCUMENT NUMBER: 124:30376
TITLE: Kemp's triacid scaffolding for synthesis of combinatorial nonpeptide uncoded libraries
AUTHOR(S): Kocis, Petr; Issakova, Olga; Sepetov, Nikolai F.; Lebl, Michal
CORPORATE SOURCE: Chem. Dep., Selectide Corp., Tucson, AZ, 85737, USA
SOURCE: Tetrahedron Letters (1995), 36(37), 6623-6
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal

102(b)

LANGUAGE: English
OTHER SOURCE(S): CASREACT 124:30376
GI



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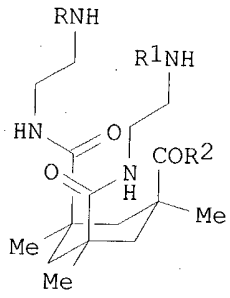


II

AB Synthesis of differentially protected mol. scaffold I (Boc = Me3CO2C; Fmoc = 9-fluorenylmethoxycarbonyl) for nonpeptide combinatorial libraries is described. Solid phase synthesis of model compds. II [R = PhCH2CH2CO, R1 = Ac, R3 = Lys(Admoc)-OH; R = Ac-Phe, R1 = Ac, R2 = Arg-.beta.-Ala-Gly-.beta.-Ala-Gly-OH; R = 6-amino-3-pyridinecarbonyl, R1 = 4-[HN:C(NH2)NH]C6H4CO, R2 = Arg-.beta.-Ala-Gly-.beta.-Ala-Gly-OH; R = HO2CCH2CH2CO, R1 = 2-pyrazinecarbonyl, R2 = Asp-.beta.-Ala-Gly-.beta.-Ala-Gly-OH; Admoc = 1-adamantylmethoxycarbonyl] and a nonpeptide combinatorial library as well as the structure elucidation in the absence of coding is disclosed.

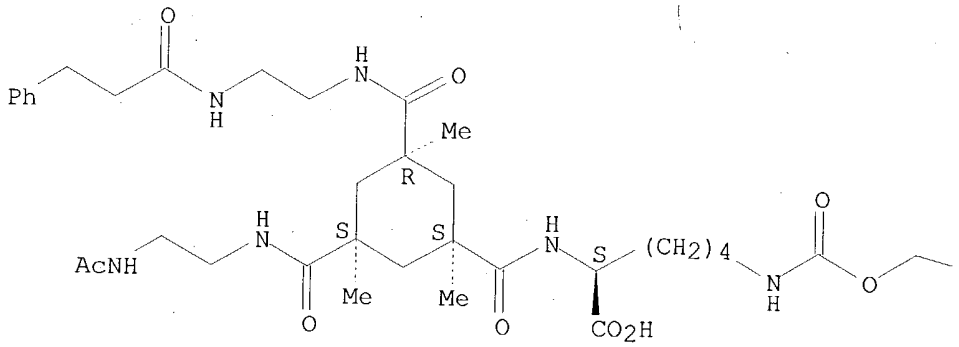
IT **171563-25-0P 171563-26-1P 171563-27-2P**
171563-28-3P 171563-30-7DP, diamide reaction products with carboxylic acid mixts.
RL: SPN (Synthetic preparation); PREP (Preparation)
(use of Kemp's triacid as a scaffold for the prepn. of nonpeptide uncoded combinatorial libraries)

RN 171563-25-0 HCAPLUS

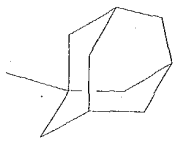
CN L-Lysine, N2-[[3-[[[2-(acetylamino)ethyl]amino]carbonyl]-1,3,5-trimethyl-5-[[[2-[(1-oxo-3-phenylpropyl)amino]ethyl]amino]carbonyl]cyclohexyl]carbonyl]-N6-[(tricyclo[3.3.1.13,7]dec-1-ylmethoxy)carbonyl]-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



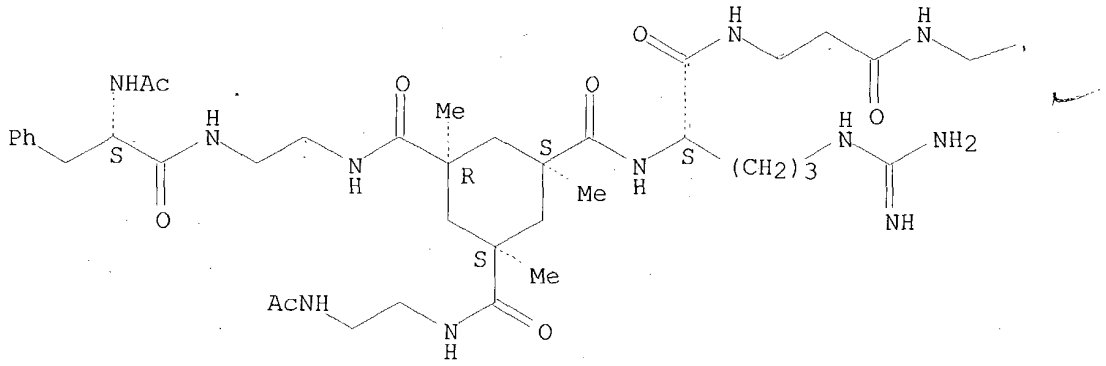
PAGE 1-B



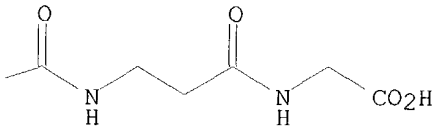
RN 171563-26-1 HCAPLUS
CN Glycine, N-[N-[N-[N-[N2-[[3-[[[2-(acetylamino)ethyl]amino]carbonyl]-5-[[[2-[[2-(acetylamino)-1-oxo-3-phenylpropyl]amino]ethyl]amino]carbonyl]-1,3,5-trimethylcyclohexyl]carbonyl]-L-arginyl]-.beta.-alanyl]glycyl]-.beta.-alanyl]-, [1S-[1.alpha.,3.alpha.,5.alpha.(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



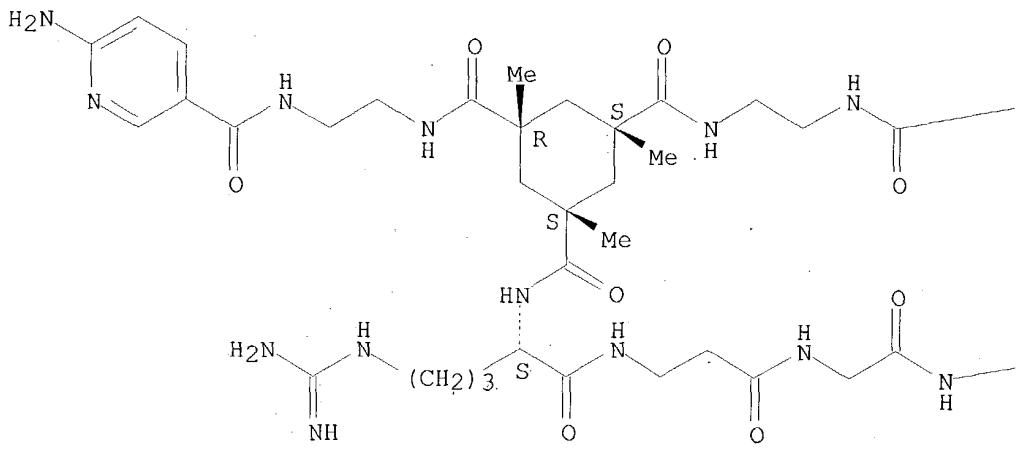
PAGE 1-B



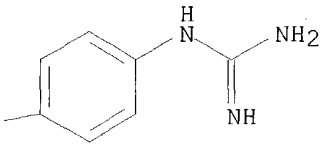
RN 171563-27-2 HCAPLUS
CN Glycine, N-[N-[N-[N-[N2-[[3-[[[2-[[4-[(aminoiminomethyl)amino]benzoyl]amino]ethyl]amino]carbonyl]-5-[[[2-[[(6-amino-3-pyridinyl)carbonyl]amino]ethyl]amino]carbonyl]-1,3,5-trimethylcyclohexyl]carbonyl]-L-arginyl]-.beta.-alanyl]glycyl]-.beta.-alanyl]-, [1S-(1.alpha.,3.alpha.,5.alpha.)]- (9CI) (CA INDEX NAME)

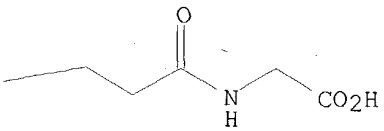
Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

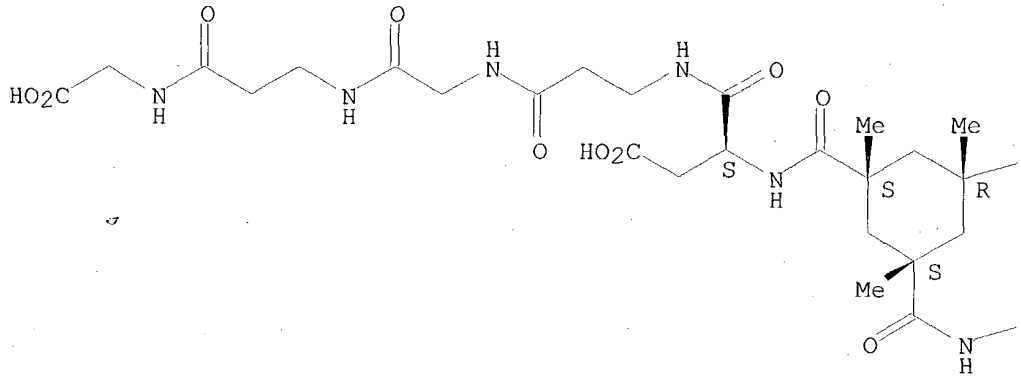




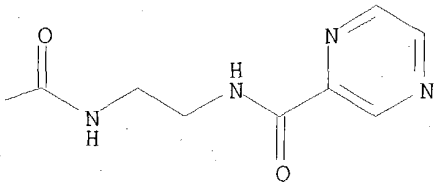
RN 171563-28-3 HCAPLUS
CN Glycine, N-[N-[N-[N-[[3-[[[2-[(3-carboxy-1-oxopropyl)amino]ethyl]amino]carbonyl]-1,3,5-trimethyl-5-[[[2-[(pyrazinylcarbonyl)amino]ethyl]amino]carbonyl]cyclohexyl]carbonyl]-L-.alpha.-aspartyl]-.beta.-alanyl]glycyl]-.beta.-alanyl]-, [1S-(1.alpha.,3.alpha.,5.alpha.)]- (9CI) (CA INDEX NAME)

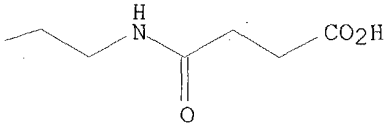
Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

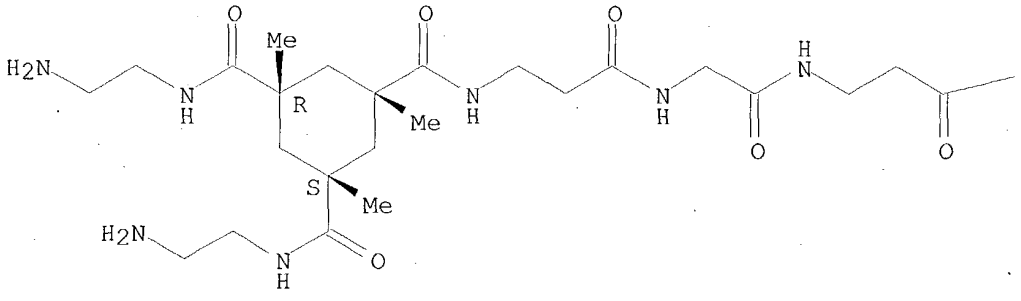


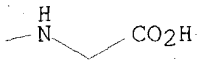


RN 171563-30-7 HCAPLUS
CN Glycine, N-[N-[N-[N-[[3,5-bis[[(2-aminoethyl)amino]carbonyl]-1,3,5-trimethylcyclohexyl]carbonyl]-.beta.-alanyl]glycyl]-.beta.-alanyl]-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



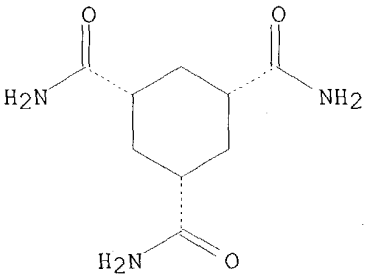


L27 ANSWER 47 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1995:654302 HCAPLUS
DOCUMENT NUMBER: 123:228292
TITLE: Synthesis and complexation behavior of the functionalized tripodal phosphine cis,cis-1,3,5-tris(cyano)-1,3,5-tris(diphenylphosphinyl)cyclohexane (tdppcycn)
AUTHOR(S): Mayer, Hermann A.; Stoessel, Philipp; Fawzi, Riad; Steimann, Manfred
CORPORATE SOURCE: Institut Anorganische Chemie, Universitaet Tuebingen, Tuebingen, D-72076, Germany
SOURCE: Chemische Berichte (1995), 128(7), 719-23
CODEN: CHBEAM; ISSN: 0009-2940
PUBLISHER: VCH
DOCUMENT TYPE: Journal
LANGUAGE: English

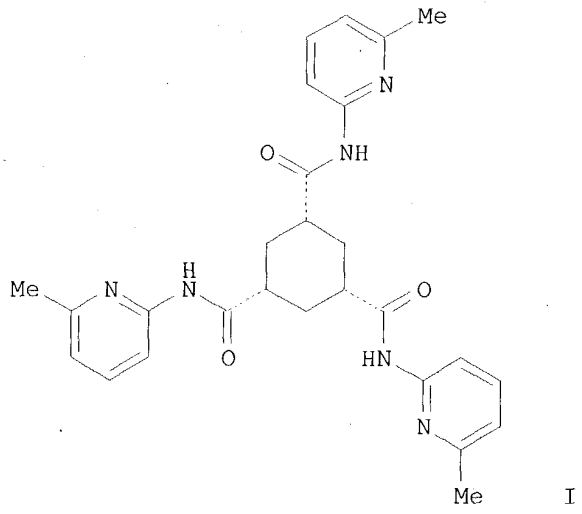
AB The synthesis of the novel potentially bistripodal ligand cis-cis-1,3,5-tris(cyano)-1,3,5-tris(diphenylphosphanyl)cyclohexane (tdppcycn) (6) is described. Starting from the tricarboxylic acid cis,cis-1,3,5-C6H9(COOH)3 (1), which is converted stepwise into the triacid chloride cis,cis-1,3,5-C6H9(COCl)3 (2), the tri-Ph ester cis,cis-1,3,5-C6H9(COOPh)3 (3), the tricarboxamide cis,cis-1,3,5-C6H9(CONH2)3 (4), and the tricarbonitrile cis,cis-1,3,5-C6H9(CN)3 (5); tdppcycn (6) was prepd. by .alpha.-deprotonation of 5 followed by treatment with ClPPh2 in good yield. Treatment of 6 with Mo(CO)3(.eta.6-C7H8) and Ir(PPh3)2(CO)Cl gave octahedral Mo(tdppcycn)(CO)3 (7) and pentacoordinate Ir(tdppcycn)(CO)Cl (8), resp., with a facially P-coordinated tdppcycn ligand. The stereochem. of compds. 2-8 was established by 1H-, 13C-, 31P-NMR, and IR spectroscopy. An x-ray crystal structure anal. of complex 8 confirms the trigonal-bipyramidal ground-state structure in the solid state.

IT **168280-45-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction with thionyl chloride in presence of DMF)
RN 168280-45-3 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L27 ANSWER 48 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1995:644496 HCAPLUS
DOCUMENT NUMBER: 123:284942
TITLE: Hydrogen-bonding control of molecular aggregation: self-complementary subunits lead to rod-shaped structures in the solid state
AUTHOR(S): Fan, Erkang; Yang, Ji; Geib, Steven J.; Stoner, Timothy C.; Hopkins, Michael D.; Hamilton, Andrew D.
CORPORATE SOURCE: Dep. Chem., Univ. Pittsburgh, Pittsburgh, PA, 15260, USA
SOURCE: Journal of the Chemical Society, Chemical Communications (1995), (12), 1251-2
CODEN: JCCCAT; ISSN: 0022-4936
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



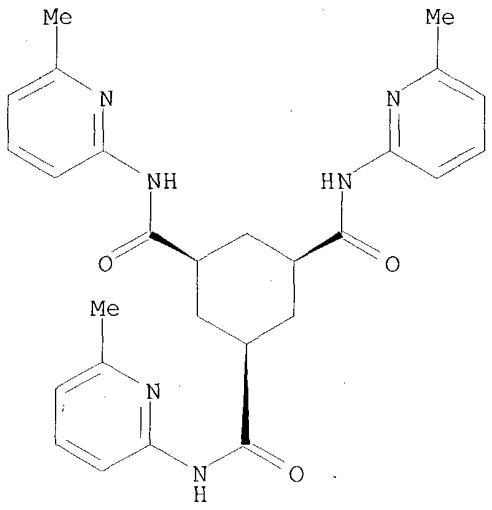
I

AB Simple cyclohexane-1,3,5-triamide derivs. (e.g. I) are shown to form linear, rod-shaped structures in the solid state; a triple hydrogen-bonding interaction directs formation of the aggregate and leads to non-centrosym. packing arrangement with modest nonlinear optical properties.

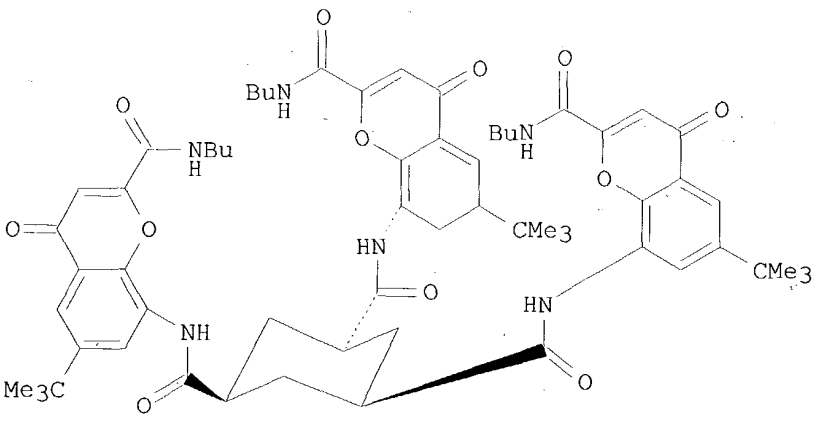
IT **169557-72-6**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(hydrogen-bonding control of mol. aggregation in cyclohexane-1,3,5-triamide derivs.)

RN 169557-72-6 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris(6-methyl-2-pyridinyl)-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L27 ANSWER 49 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1995:550045 HCAPLUS
DOCUMENT NUMBER: 123:256099
TITLE: A cyclohexane spacer for phosphate receptors
AUTHOR(S): Raposo, Cesar; Perez, Nieves; Almaraz, Marta; Mussons, M. Luisa; Caballero, M. Cruz; Moran, Joaquin R.
CORPORATE SOURCE: Dep. Quim. Org., Univ. Salamanca, Salamanca, E-37008, Spain
SOURCE: Tetrahedron Letters (1995), 36(18), 3255-8
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB A cyclohexanetricarboxylic acid is shown to be a good spacer for phosphate guests. The combination of 8-aminochromenone-2-carboxamide groups with the cyclohexane spacer leads to a versatile receptor (I), which sets six hydrogen bonds with either phosphonic acids or phosphates. Large assocn. consts. are obtained for this receptor in DMSO and methanol when tetraalkylammonium phosphates are used as guests.

IT **168705-28-0P**

RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(hydrogen bonded with phenylphosphonic acid; cyclohexane spacer for phosphate receptors)

RN 168705-28-0 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris[2-[(butylamino)carbonyl]-6-(1,1-dimethylethyl)-4-oxo-4H-1-benzopyran-8-yl]-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

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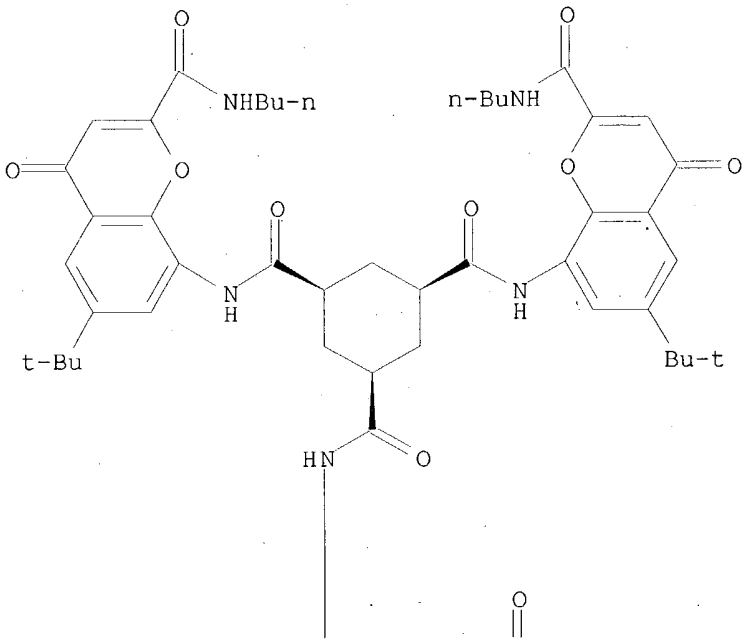

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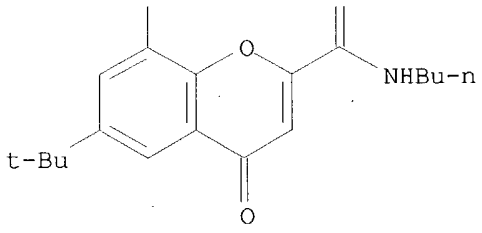


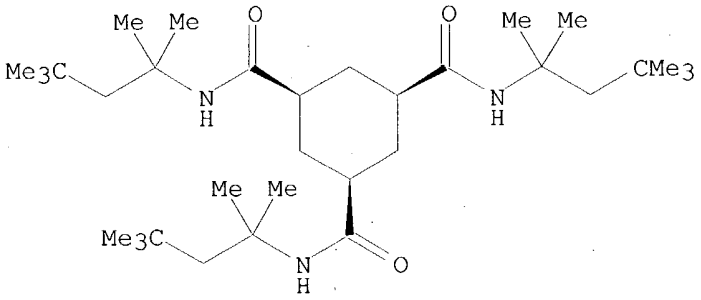
IT **168705-27-9P**

RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(hydrogen bonded with propylphosphonic acid; cyclohexane spacer for phosphate receptors)

RN 168705-27-9 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tris(1,1,3,3-tetramethylbutyl)-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

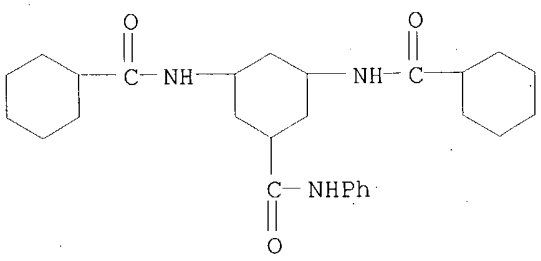
Relative stereochemistry.



L27 ANSWER 50 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1995:543429 HCAPLUS
DOCUMENT NUMBER: 122:267113
TITLE: Polyamide and amide compound compositions with good degree of crystallinity
INVENTOR(S): Kitagawa, Hiroshi; Yana, Yoshitaka; Mizoguchi, Kazuaki; Kawahara, Yasuyuki; Sadamitsu, Kyoshi; Yoshimura, Masafumi; Ikeda, Naoki
PATENT ASSIGNEE(S): Shin Nippon Rika KK, Japan; New Japan Chemical Co., Ltd.
SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06271762	A2	19940927	JP 1994-15830	19940113
JP 3477787	B2	20031210		
JP 2004035895	A2	20040205	JP 2003-290992	20030811

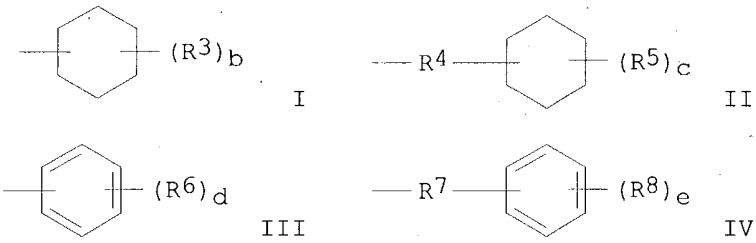
PRIORITY APPLN. INFO.: JP 1993-26179 A 19930120
JP 1994-15830 A3 19940113
OTHER SOURCE(S): MARPAT 122:267113
AB The compns. comprise a polyamide and a compd. selected from polycarboxylic acid amide, polyamine polyamide and/or polyamino amide. A compn. from nylon 6 contg. 0.2 phr N,N'-dicyclohexylterephthalamide showed degree of crystallinity 182.degree..
IT **162957-51-9**
RL: MOA (Modifier or additive use); TEM (Technical or engineered material use); USES (Uses)
(polyamide and amide compd. compns. with good degree of crystallinity)
RN 162957-51-9 HCAPLUS
CN Cyclohexanecarboxamide, 3,5-bis[(cyclohexylcarbonyl)amino]-N-phenyl- (9CI) (CA INDEX NAME)



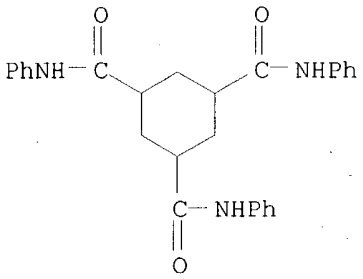
L27 ANSWER 51 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1995:118642 HCAPLUS
DOCUMENT NUMBER: 122:107612
TITLE: Crystalline propylene polymer compositions with excellent rigidity
INVENTOR(S): Mizoguchi, Kazuaki; Yoshimura, Masafumi; Ikeda, Naoki; Sadamitsu, Kyoshi; Kawahara, Yasuyuki; Yana, Yoshitaka; Kitagawa, Hiroshi
PATENT ASSIGNEE(S): Shin Nippon Rika Kk, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06192496	A2	19940712	JP 1993-269840	19930930
JP 3401868	B2	20030428		

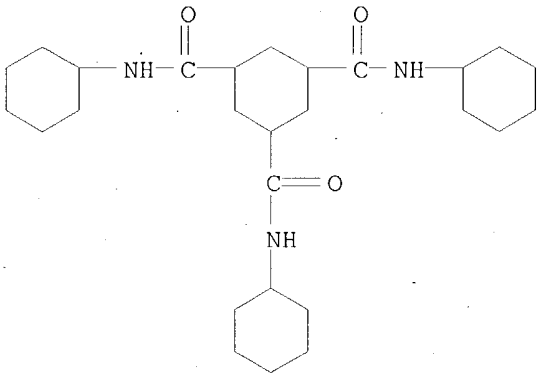
PRIORITY APPLN. INFO.: JP 1992-308233 A1 19921022
GI



AB The compns. contain .gtoreq.1 R1(CONHR2)a [R1 = aliph., alicyclic, or arom. polycarboxylic acid residue; R2 = (cyclo)alkyl, (cyclo)alkenyl, Ph, naphthyl, I, II, III, IV; R3, R5, R6, R8 = independently (cyclo)alkyl, alkenyl, alkoxy, Ph, halo; R4, R7 = linear or branched alkylene; a = 3-6; b, d = 1-5; c, e = 0-5]. Thus, 100 parts ethylene-propylene block copolymer (melt flow rate 2 g/10-min) and 0.2 part biphenyltetracarboxylic acid tetracyclohexylamide were melt kneaded and pelletized to give a compn. showing crystn. temp. 125.degree. for its press sheet and flexural modulus 11,300 kg/cm2 for its injection molded test piece.
IT **160535-62-6 160535-63-7**
RL: MOA (Modifier or additive use); USES (Uses)
(amide additives for rigid cryst. propylene polymers)
RN 160535-62-6 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-triphenyl- (9CI) (CA INDEX NAME)



RN 160535-63-7 HCAPLUS
CN 1,3,5-Cyclohexanetricarboxamide, N,N',N''-tricyclohexyl- (9CI) (CA INDEX NAME)

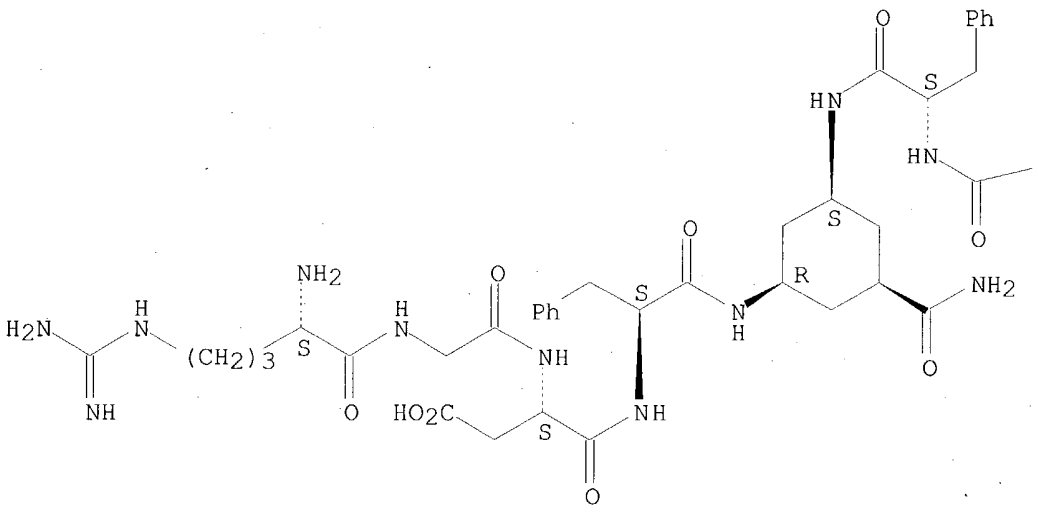


L27 ANSWER 52 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1995:32622 HCAPLUS
DOCUMENT NUMBER: 122:31918
TITLE: Structure-activity relationships of double-strand RGD peptides as GPIIb/IIIa receptor antagonists
AUTHOR(S): Ojima, Iwao; Dong, Qing; Eguchi, Masakatsu; Oh, Young-im; Amann, Clare M.; Coller, Barry S.
CORPORATE SOURCE: School. Medicine, State University New York, Stony Brook, NY, 11794, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (1994), 4(14), 1749-54
CODEN: BMCLE8; ISSN: 0960-894X
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A series of new double-strand RGD peptides M(CO-Arg-Gly-Asp-Phe-OH)2 [M = (CH2)n, p-C6H4, n = 2-4] and (R-Arg-Gly-Asp-Phe-NH)2XZ [R = H, Me(CH2)4CO, Bz, 4-[HN:C(NH2)NH]C6H4CO-Ser; X = Lys, Orn, cis,cis-3,5-diaminocyclohexanecarbonyl, 3,5-(Gly-NH)2C6H3CO; Z = NH2, Gly-Arg-Gly-Asp-Phe-NH2, Arg-Gly-Asp-Phe-OH] were prepd. and their inhibitory activities evaluated for platelet aggregation. Substantial improvement in activity is obsd. with these novel RGD peptides in comparison with single-strand RGD peptides. The structure-activity relationships of these double-strand RGD peptides are discussed.
IT **159652-31-0P 159652-32-1P 159652-33-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and blood platelet aggregation inhibitory activity of)
RN 159652-31-0 HCAPLUS
CN L-Phenylalaninamide, L-arginylglycyl-L-.alpha.-aspartyl-N-[3-

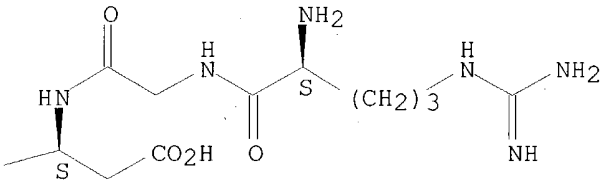
(aminocarbonyl)-5-[[N-[N-(N-L-arginylglycyl)-L-.alpha.-aspartyl]-L-phenylalanyl]amino]cyclohexyl]-, [1R-(1.alpha.,3.alpha.,5.alpha.)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

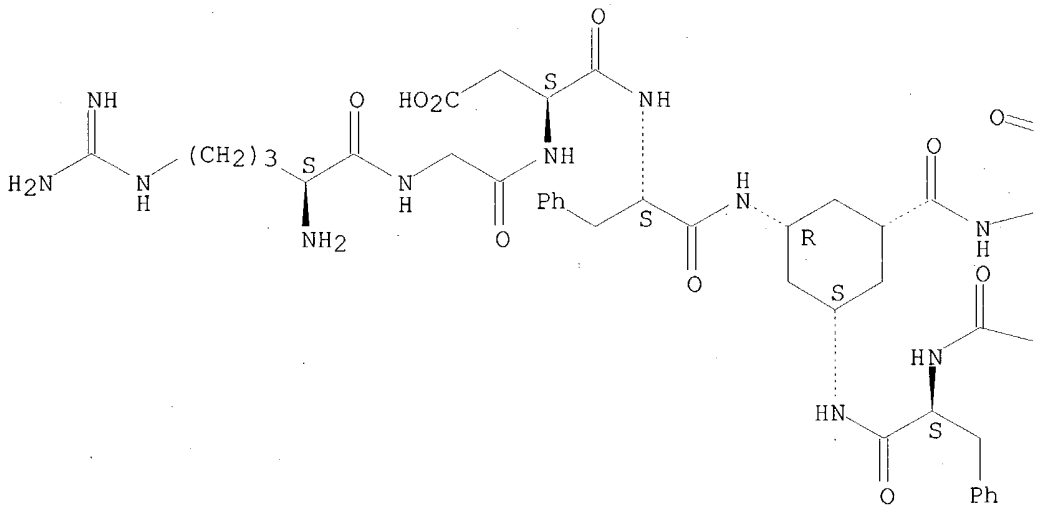


RN 159652-32-1 HCAPLUS

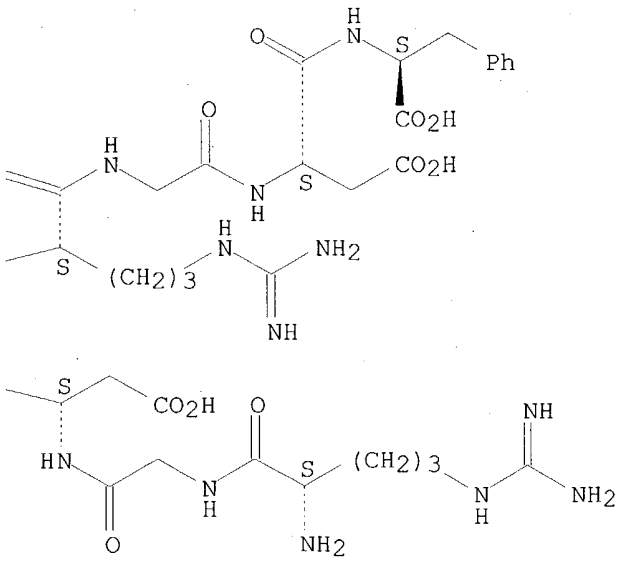
CN L-Phenylalanine, N-[N-[N-[N2-[[3,5-bis[[N-[N-(N-L-arginylglycyl)-L-.alpha.-aspartyl]-L-phenylalanyl]amino]cyclohexyl]carbonyl]-L-arginyl]glycyl]-L-.alpha.-aspartyl]-, [3R-(1.alpha.,3.alpha.,5.alpha.)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



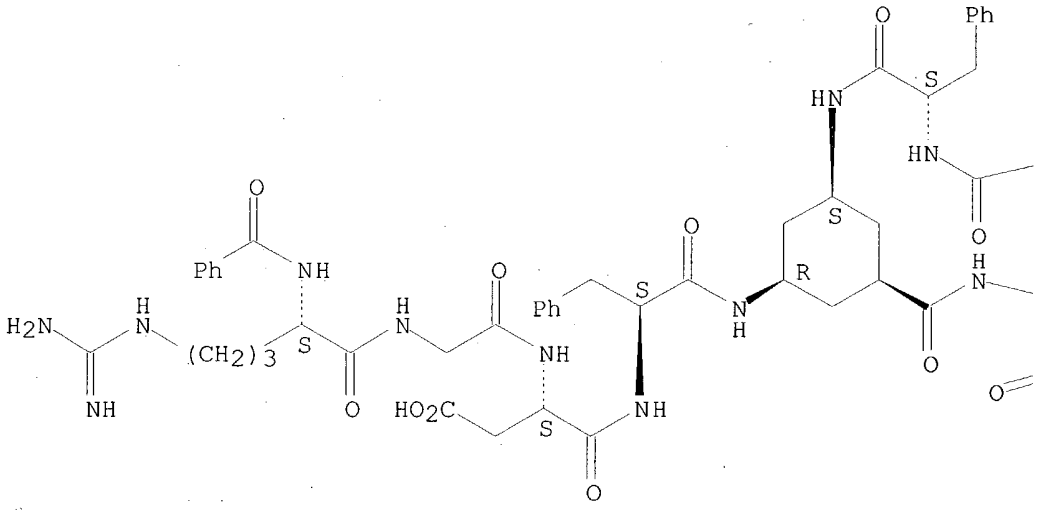
PAGE 1-B



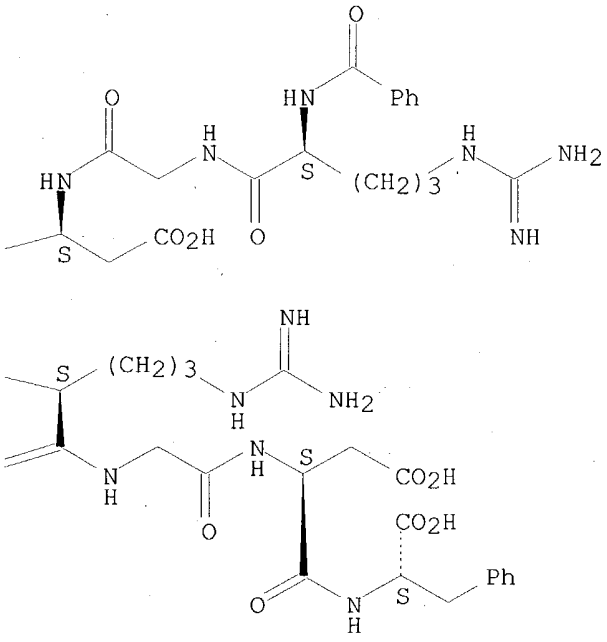
RN 159652-33-2 HCAPLUS
CN L-Phenylalanine, N-[N-[N-[N2-[[3,5-bis[[N-[N-[N-(N2-benzoyl-L-arginyl)glycyl]-L-.alpha.-asparty]-L-phenylalanyl]amino]cyclohexyl]carbonyl]-L-arginyl]glycyl]-L-.alpha.-asparty]-, [3R-(1.alpha.,3.alpha.,5.alpha.)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



L27 ANSWER 53 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1994:208601 HCAPLUS
DOCUMENT NUMBER: 120:208601
TITLE: Platelet aggregation inhibitors that prevent the interaction of platelets and fibrinogen
INVENTOR(S): Ojima, Iwao; Eguchi, Masakatsu; Oh, Young Im; Coller, Barry S.

PATENT ASSIGNEE(S): Research Foundation of State University of New York, USA
SOURCE: PCT Int. Appl., 10 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9400144	A1	19940106	WO 1993-US6150	19930629
W: AT, AU, BB, BG, BR, CA, CH, CZ, DE, DK, ES, FI, GB, HU, JP, KP, KR, LK, LU, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SK, UA, VN				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 5338725	A	19940816	US 1992-906525	19920630
AU 9346544	A1	19940124	AU 1993-46544	19930629

PRIORITY APPLN. INFO.: US 1992-906525 19920630
WO 1993-US6150 19930629

AB Synthetic peptides contg. the RGD adhesion tripeptide are prepd. for use as platelet aggregation inhibitors. The RGD peptide is flanked by by other short peptides, optionally including a alkyl, cycloalkyl, arom., or heteroarom. terminal extensions and has reactive carboxyl and amino termini for the formation of oligomers that give high local concns. of the RGD peptide. The peptide (RGPFPG)2Dab-G-OH was synthesized by Fmoc chem. to give the TFA salt, this was converted to the acetate by ion-exchange and the acetate inhibited the ability of platelet-rich plasma to aggregate with an adjusted IC50 of 6.7.times.10-7 M. Thirty-one peptides in accordance with the invention were synthesized and their adjusted IC50's were in the range 7.6.times.10-8 - 4.4.times.10-6 M.

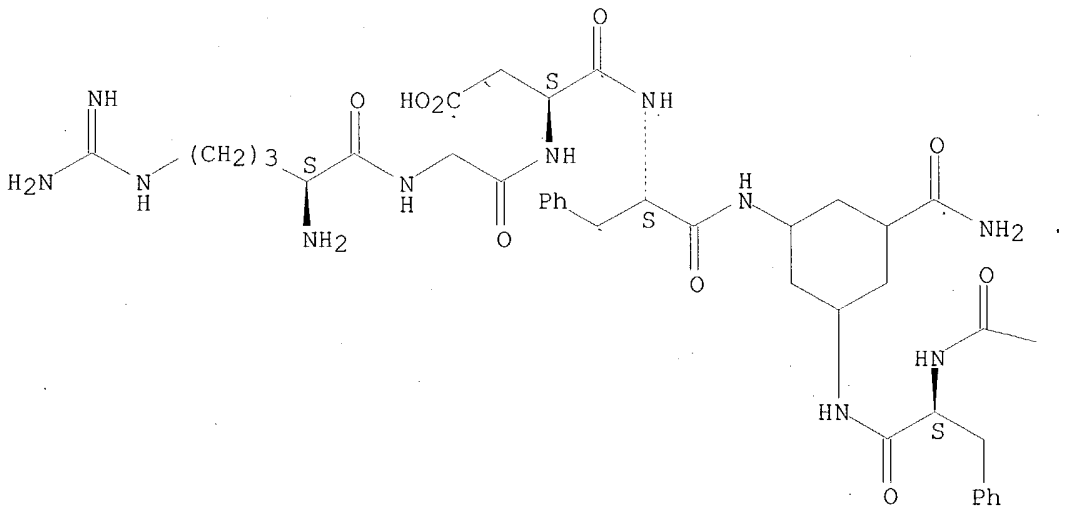
IT **154207-63-3P 154207-72-4P 154207-88-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, platelet aggregation inhibition by)

RN 154207-63-3 HCAPLUS

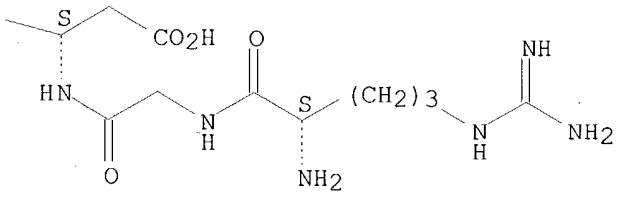
CN L-Phenylalaninamide, L-arginylglycyl-L-.alpha.-aspartyl-N-[3-(aminocarbonyl)-5-[[N-[N-(N-L-arginylglycyl)-L-.alpha.-aspartyl]-L-phenylalanyl]amino]cyclohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



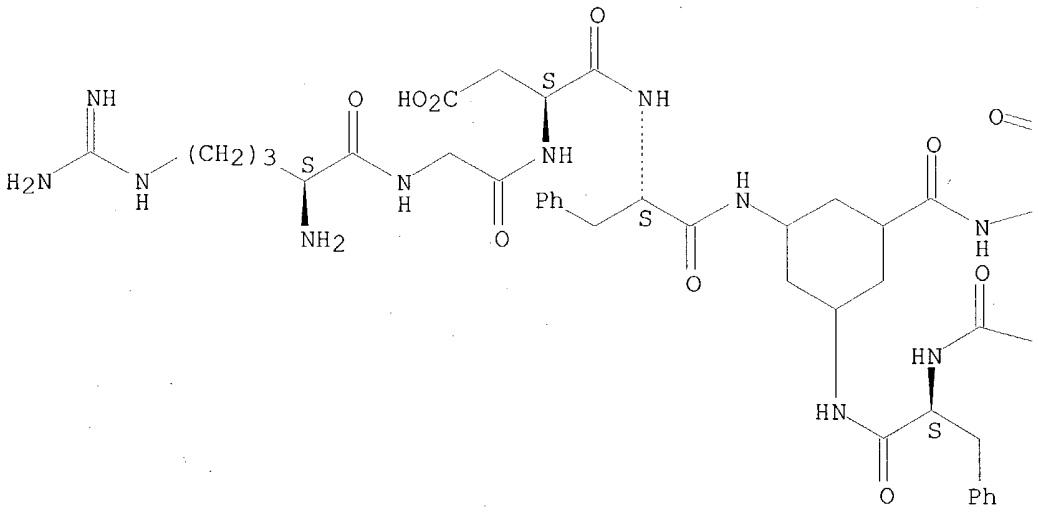
PAGE 1-B



RN 154207-72-4 HCAPLUS
CN L-Phenylalanine, N-[N-[N-[N2-[[3,5-bis[[N-[N-(N-L-arginylglycyl)-L-.alpha.-aspartyl]-L-phenylalanyl]amino]cyclohexyl]carbonyl]-L-arginyl]glycyl]-L-.alpha.-aspartyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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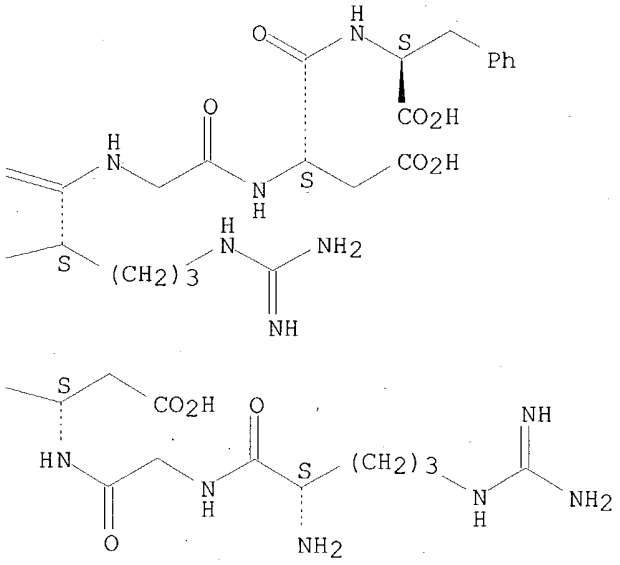
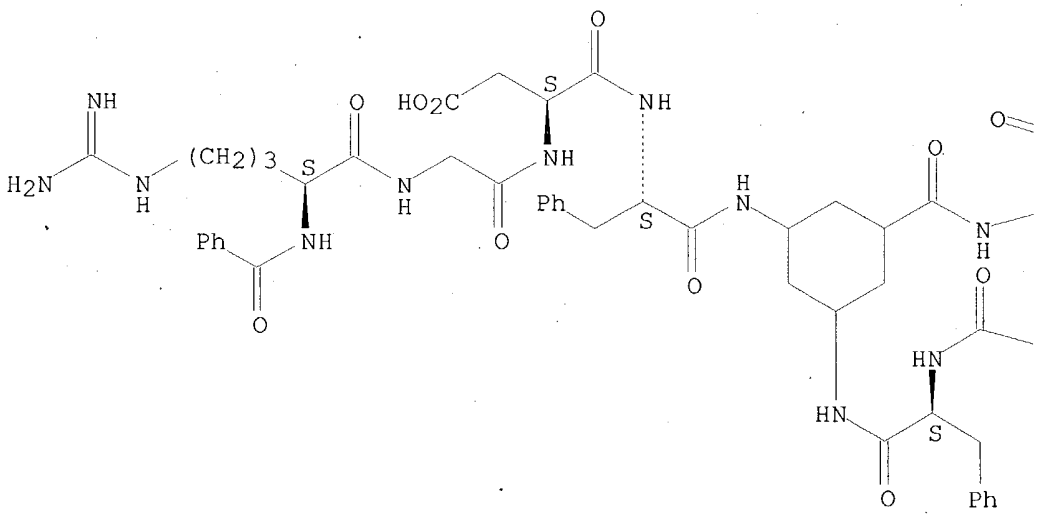


RN 154207-88-2 HCAPLUS
CN L-Phenylalanine, N-[N-[N-[N2-[[3,5-bis[[N-[N-[N-(N2-benzoyl-L-arginyl)glycyl]-L-.alpha.-aspartyl]-L-phenylalanyl]amino]cyclohexyl]carbonyl]-L-arginyl]glycyl]-L-.alpha.-aspartyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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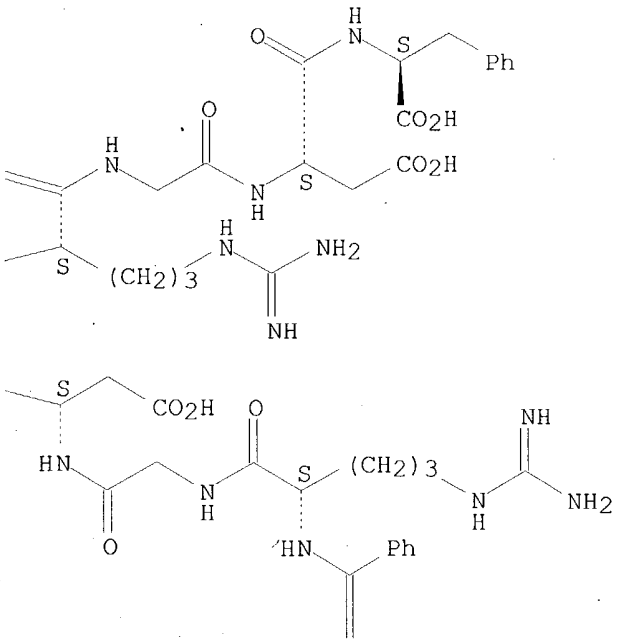

PAGE 2-B

L27 ANSWER 54 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1994:192086 HCAPLUS
DOCUMENT NUMBER: 120:192086
TITLE: Preparation of bile acid derivatives as hypolipemics
INVENTOR(S): Enhsen, Alfons; Glombik, Heiner; Kramer, Werner; Wess, Guenther
PATENT ASSIGNEE(S): Hoechst A.-G., Germany
SOURCE: Eur. Pat. Appl., 32 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 573848	A2	19931215	EP 1993-108559	19930527
EP 573848	B1	19971203		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
AT 160783	E	19971215	AT 1993-108559	19930527
ES 2111092	T3	19980301	ES 1993-108559	19930527
US 5428182	A	19950627	US 1993-74753	19930610
IL 105980	A1	19971120	IL 1993-105980	19930610
CZ 285104	B6	19990512	CZ 1993-1134	19930610
SK 280819	B6	20000814	SK 1993-585	19930610
CA 2098256	AA	19931213	CA 1993-2098256	19930611
NO 9302159	A	19931213	NO 1993-2159	19930611

AU 9340180	A1	19931216	AU 1993-40180	19930611
AU 663592	B2	19951012		
ZA 9304150	A	19940113	ZA 1993-4150	19930611
HU 64772	A2	19940228	HU 1993-1716	19930611
HU 216636	B	19990728		
JP 06087884	A2	19940329	JP 1993-140375	19930611
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PRIORITY APPLN. INFO.: DE 1992-4219274 A 19920612
OTHER SOURCE(S): MARPAT 120:192086
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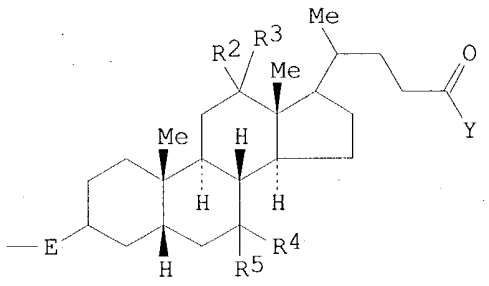
Q= 

AB Z(XG)n (G = bile acid residue, e.g., Q; E = bond, O, NH; R2-R5 = H, OH, alkoxy, NH2, alkanoyloxy, etc.; X = bond, bridging group; Y = OH, alkoxy, NH2, etc.; Z = n-valent group; n = 3 or 4) were prepd. Thus, MeC(CH2OCH2CH2COR7)3 (I; R7 = OH) was condensed with RCH2CH2NH2 (R = Q; E = .beta.-O, R2 = R4 = .alpha.-OH, R3 = R5 = H, Y = OR6)(Q1; R6 = Me) to give, after sapon., I (R7 = NHCH2CH2Q1; R6 = H) which had IC50 0.24 that of taurochenodesoxycholate for inhibition of taurocholate uptake by rabbit ileal vesicles in vitro.

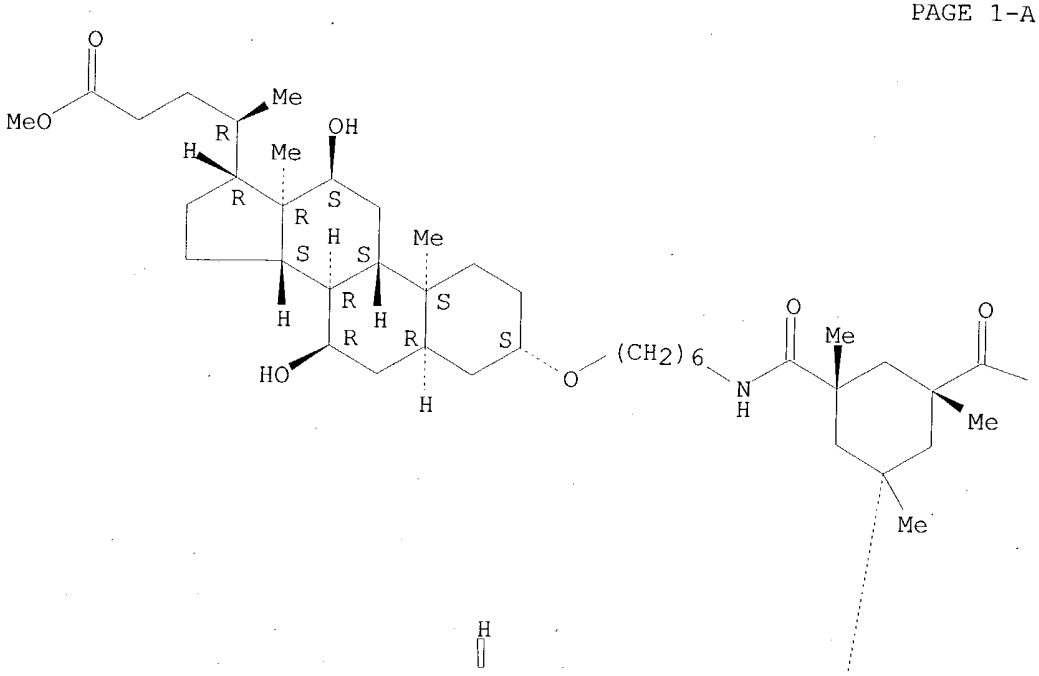
IT **153582-90-2P 153582-91-3P 153582-97-9P**
153582-98-0P 153582-99-1P 153583-03-0P
153583-04-1P 153583-05-2P 153583-06-3P
153583-07-4P 153583-08-5P 153583-09-6P
153583-11-0P 153583-12-1P 153583-13-2P
153665-88-4P 153665-89-5P 153665-90-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as hypolipemic)

RN 153582-90-2 HCAPLUS

CN Cholan-24-oic acid, 3,3',3''-[(1,3,5-trimethyl-1,3,5-cyclohexanetriyl)tris(carbonylimino-6,1-hexanediyloxy)]tris[7,12-dihydroxy-, trimethyl ester, stereoisomer (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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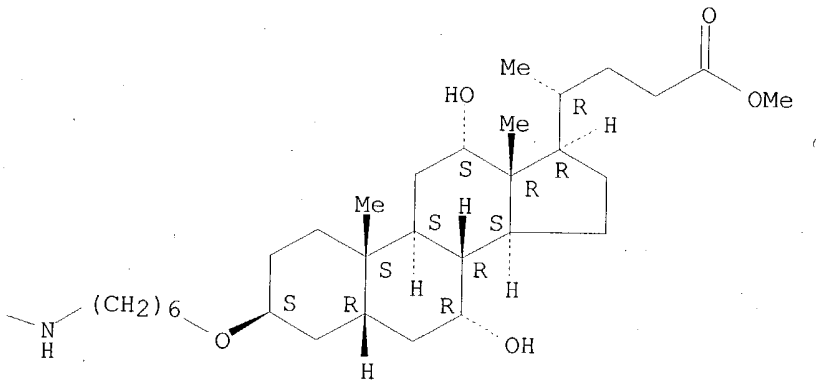
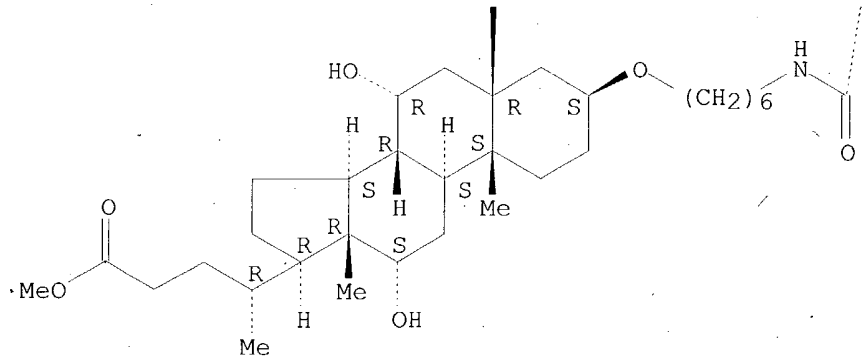


PAGE 2-A



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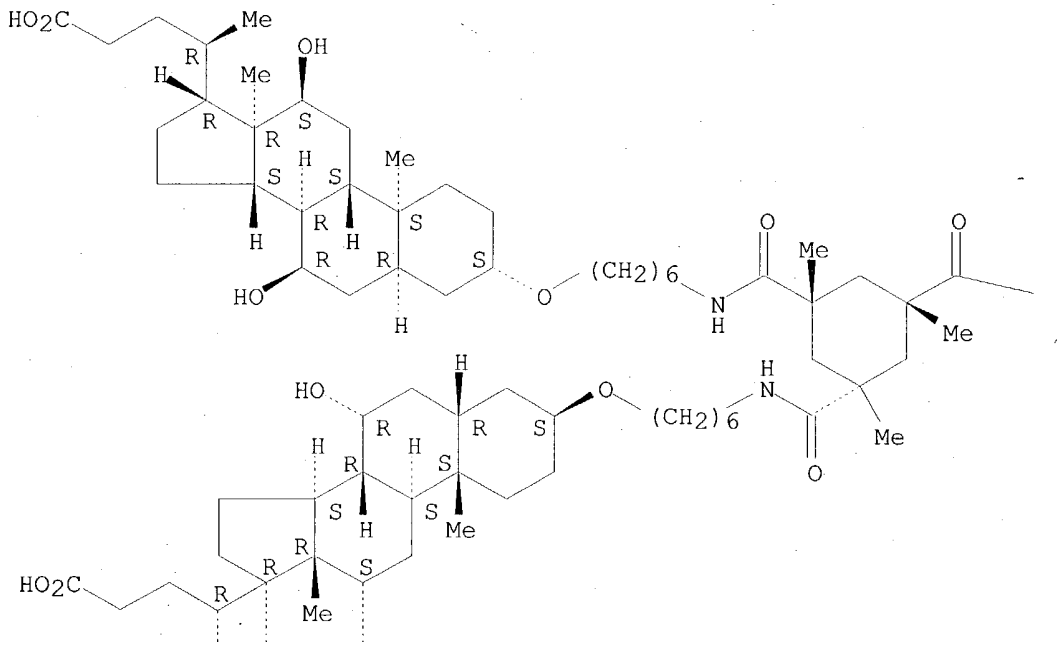
CN Cholan-24-oic acid, 3,3',3''-[(1,3,5-trimethyl-1,3,5-cyclohexanetriyl)tris(carbonylimino-6,1-hexanediyloxy)]tris[7,12-dihydroxy-, stereoisomer (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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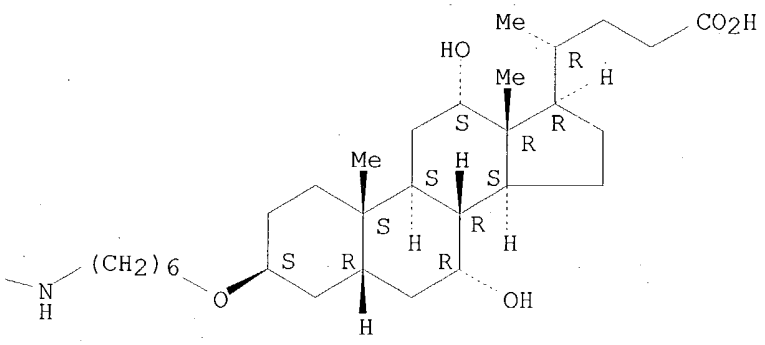

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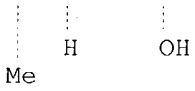
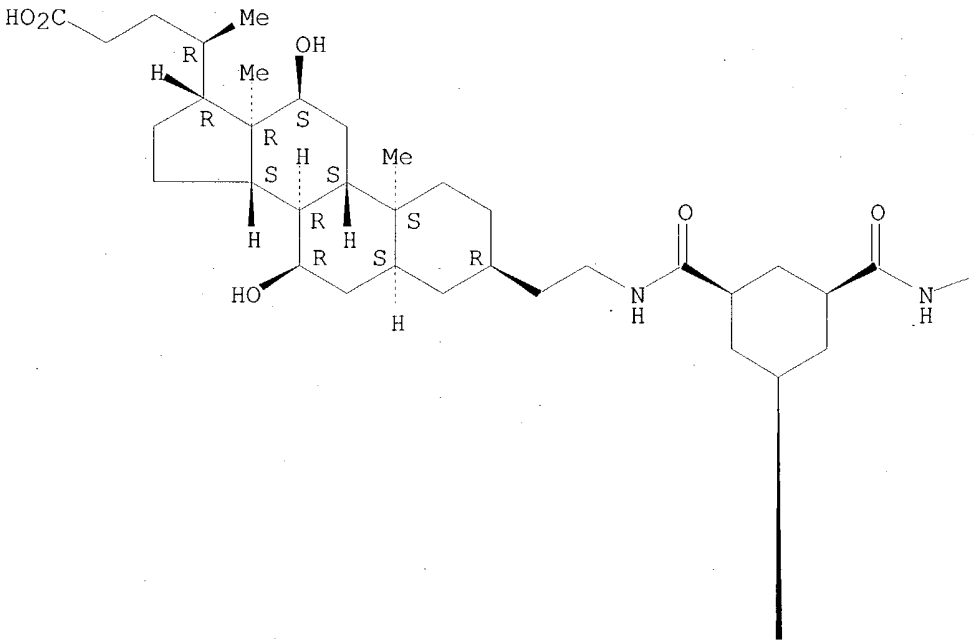


RN 153582-97-9 HCAPLUS
CN Cholan-24-oic acid, 3,3',3''-[1,3,5-cyclohexanetriyltris(carbonylimino-2,1-ethanediyl)]tris[7,12-dihydroxy-, stereoisomer (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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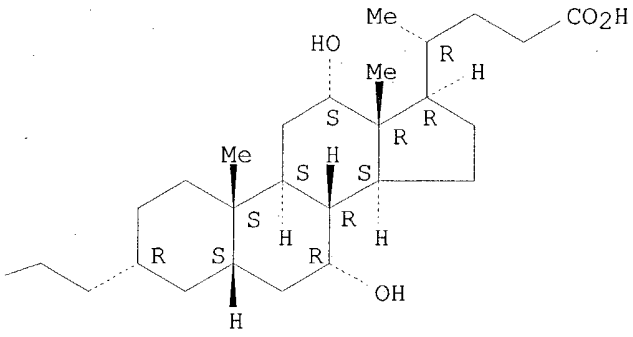

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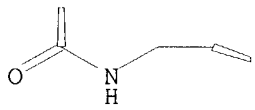
PAGE 2-A



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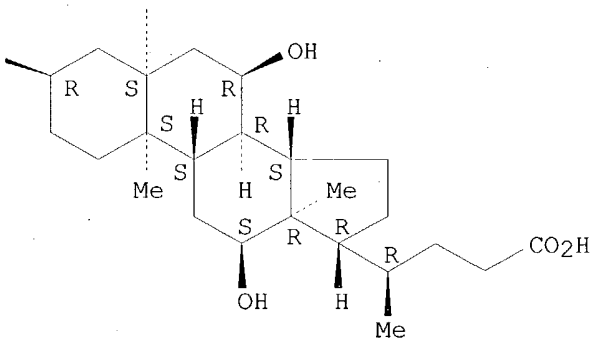
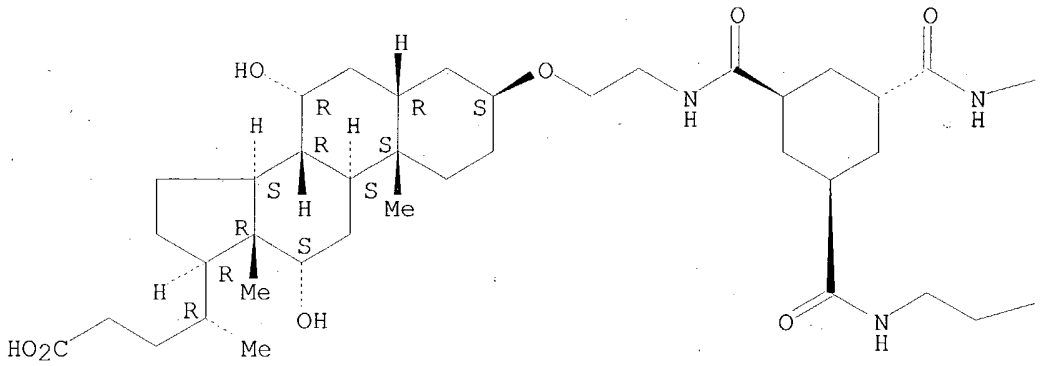


RN 153582-98-0 HCAPLUS
CN Cholan-24-oic acid, 3,3',3''-[1,3,5-cyclohexanetriyltris(carbonylimino-2,1-ethanediyloxy)]tris[7,12-dihydroxy-, stereoisomer (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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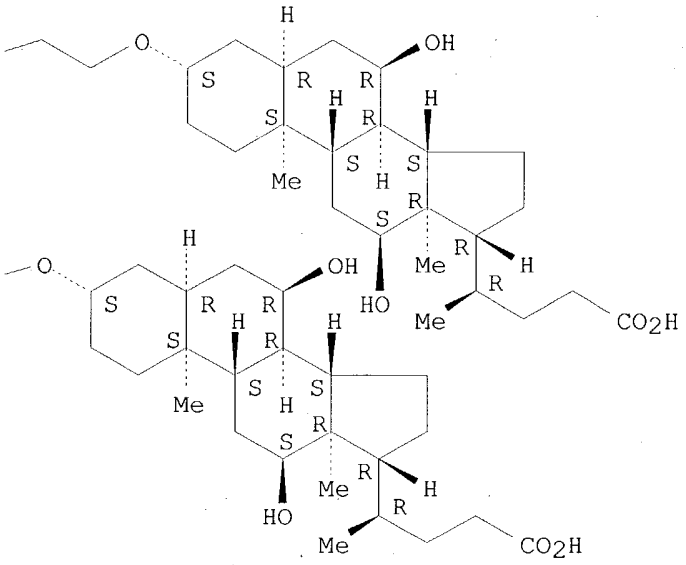
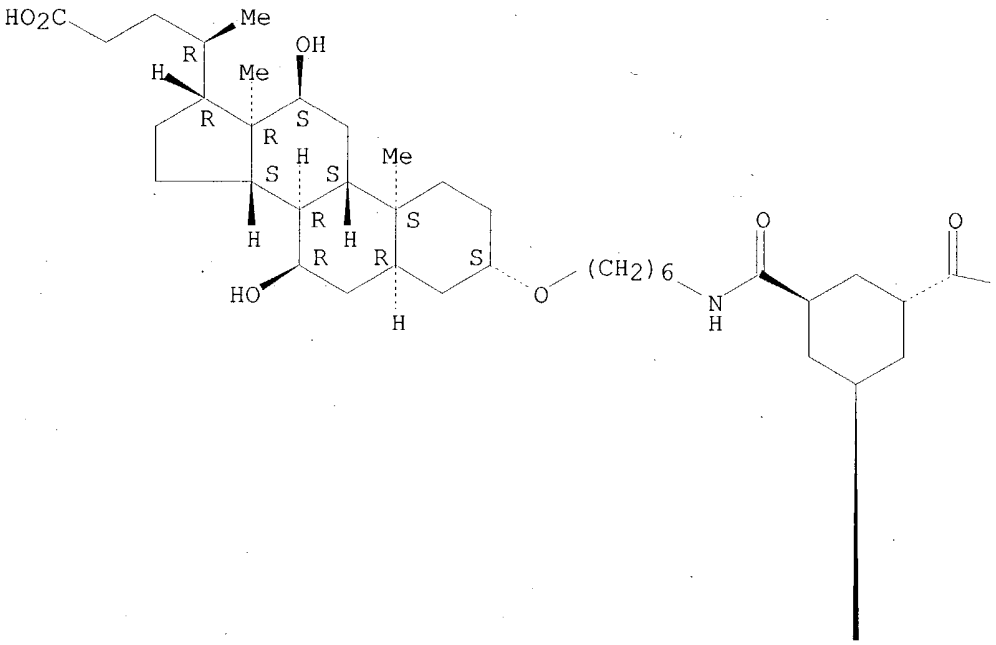


RN 153582-99-1 HCAPLUS
CN Cholan-24-oic acid, 3,3',3''-[1,3,5-cyclohexanetriyltris(carbonylimino-6,1-hexanediyloxy)]tris[7,12-dihydroxy-, stereoisomer (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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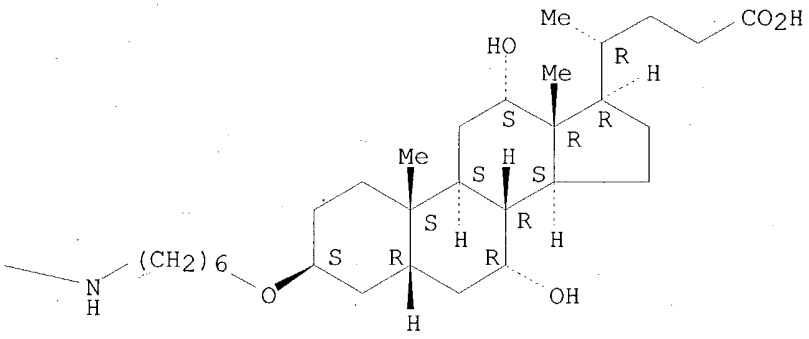

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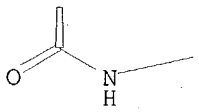

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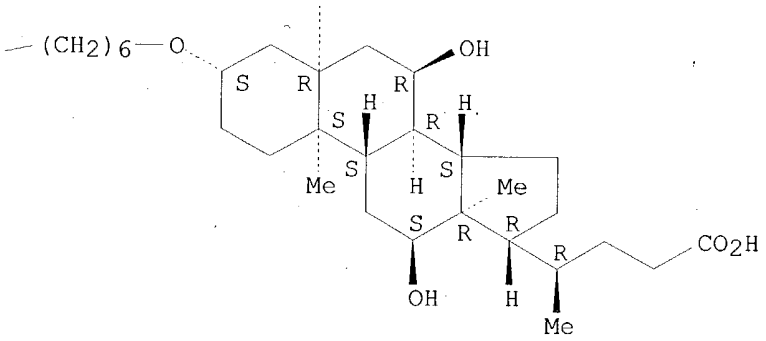

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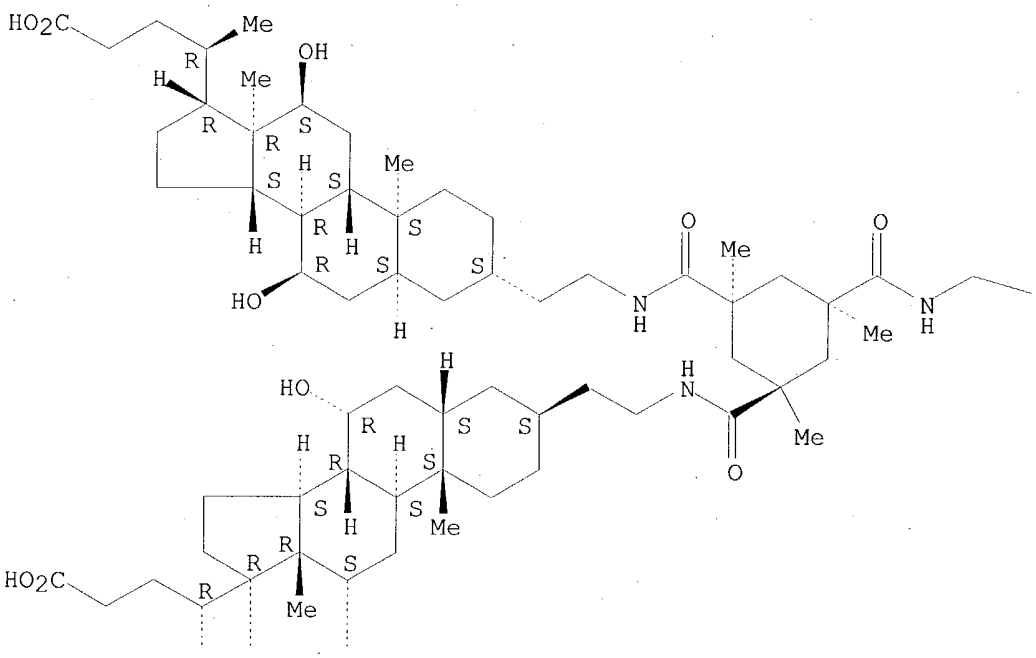
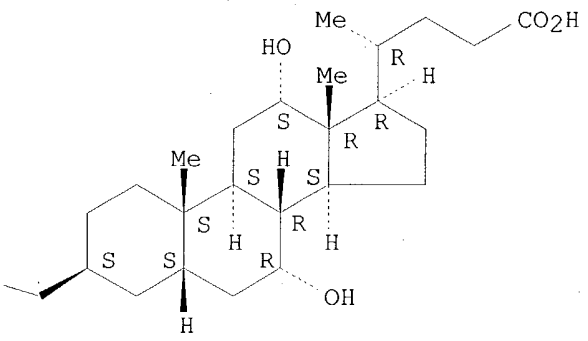
Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



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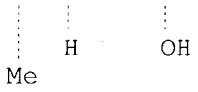
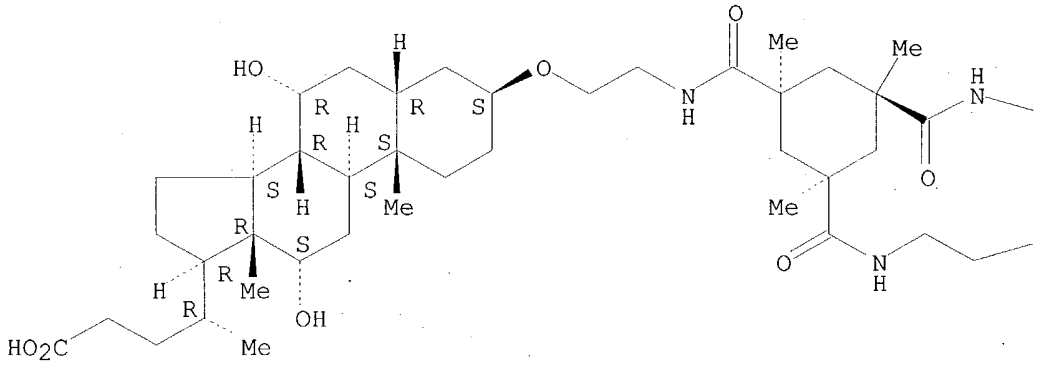


RN 153583-04-1 HCAPLUS
CN Cholan-24-oic acid, 3,3',3''-[(1,3,5-trimethyl-1,3,5-cyclohexanetriyl)tris(carbonylimino-2,1-ethanediyloxy)]tris[7,12-dihydroxy-, stereoisomer (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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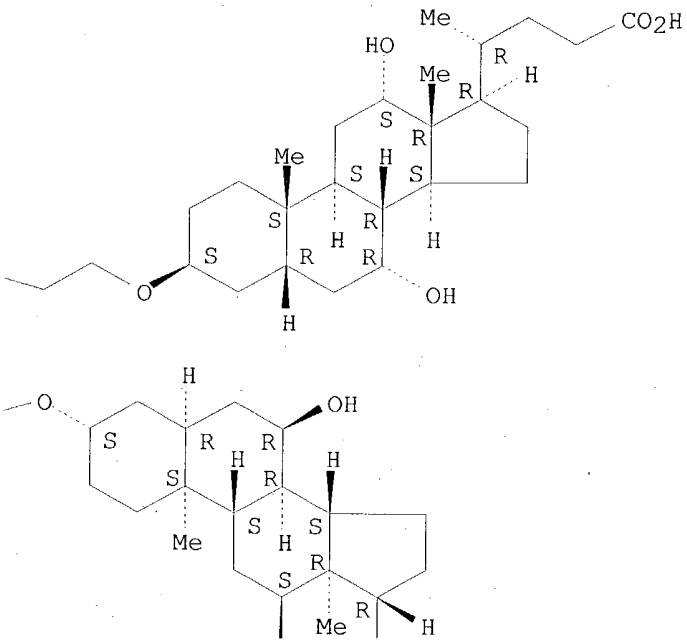

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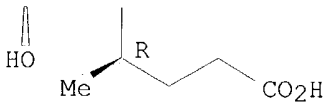

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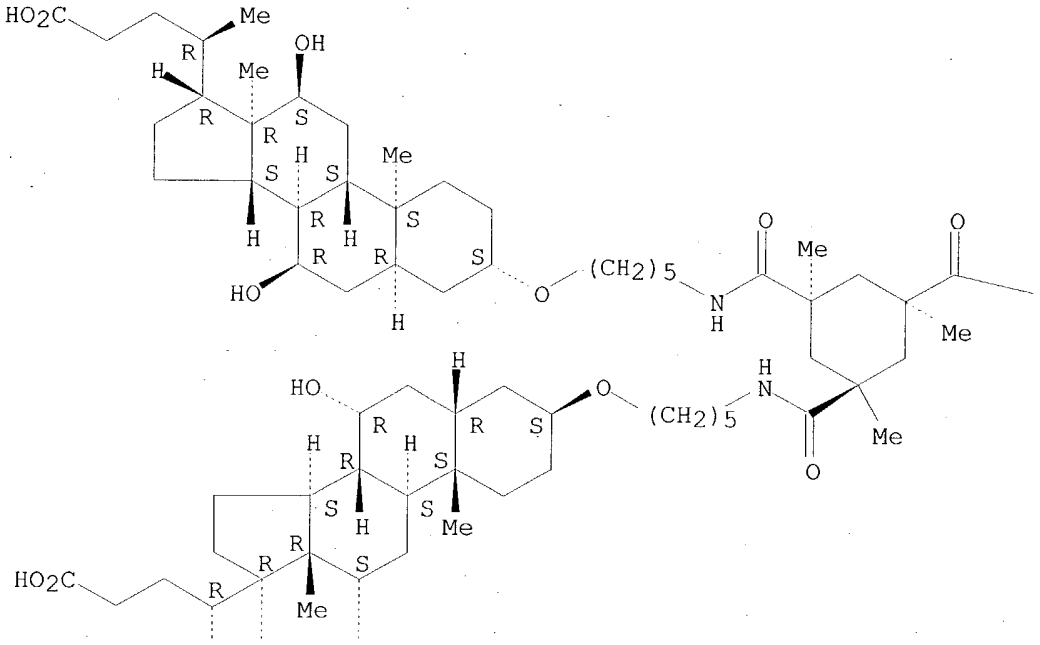
CN Cholan-24-oic acid, 3,3',3''-[(1,3,5-trimethyl-1,3,5-cyclohexanetriyl)tris(carbonylimino-5,1-pentanediyloxy)]tris[7,12-dihydroxy-, stereoisomer (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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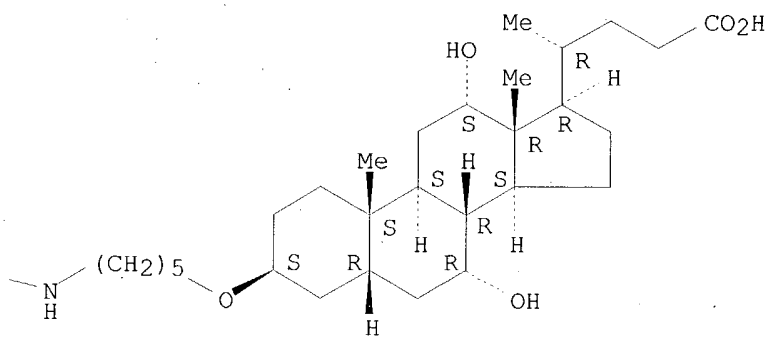

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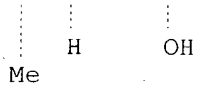
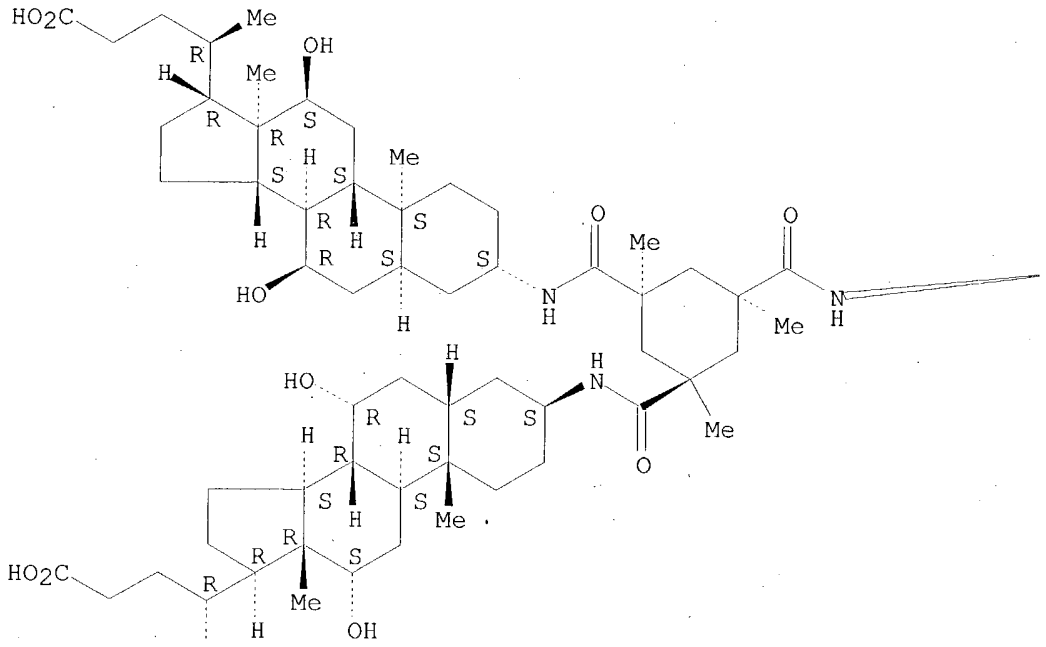


RN 153583-06-3 HCAPLUS
CN Cholan-24-oic acid, 3,3',3''-[(1,3,5-trimethyl-1,3,5-cyclohexanetriyl)tris(carbonylimino)]tris[7,12-dihydroxy-, stereoisomer (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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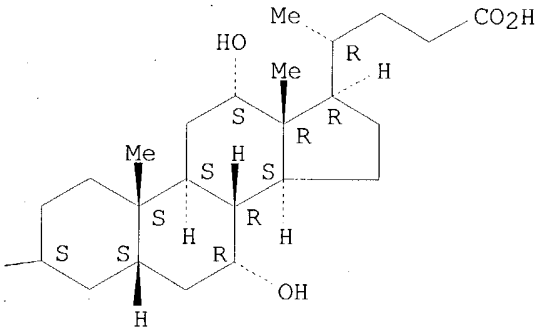

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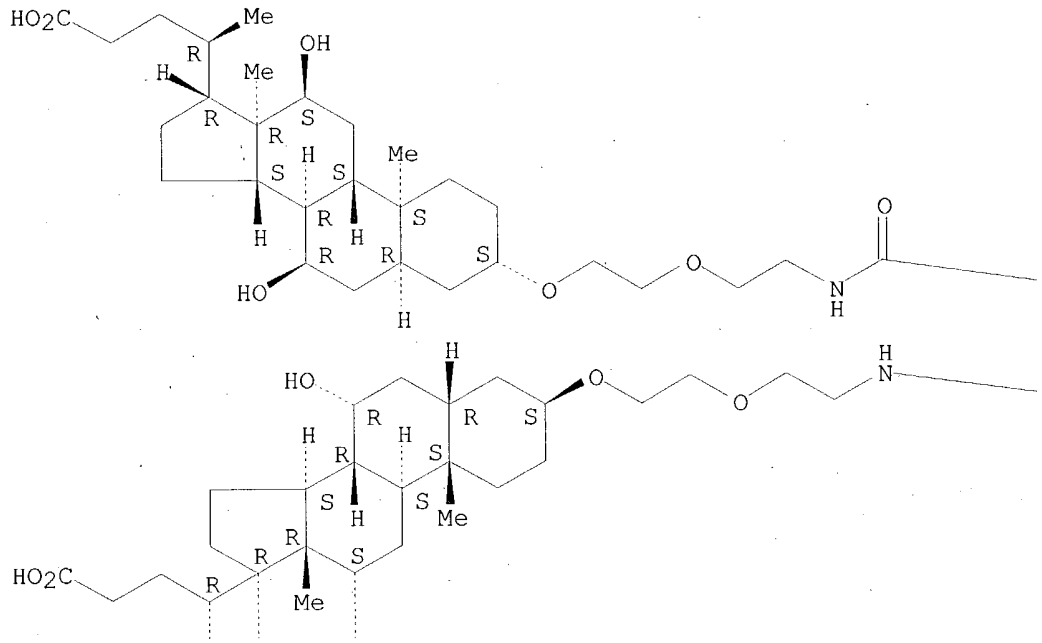
RN 153583-07-4 HCAPLUS
CN Cholan-24-oic acid, 3,3',3''-[(1,3,5-trimethyl-1,3,5-cyclohexanetriyl)tris(carbonylimino-2,1-ethanediyloxy-2,1-ethanediyloxy)]tris[7,12-dihydroxy-, stereoisomer (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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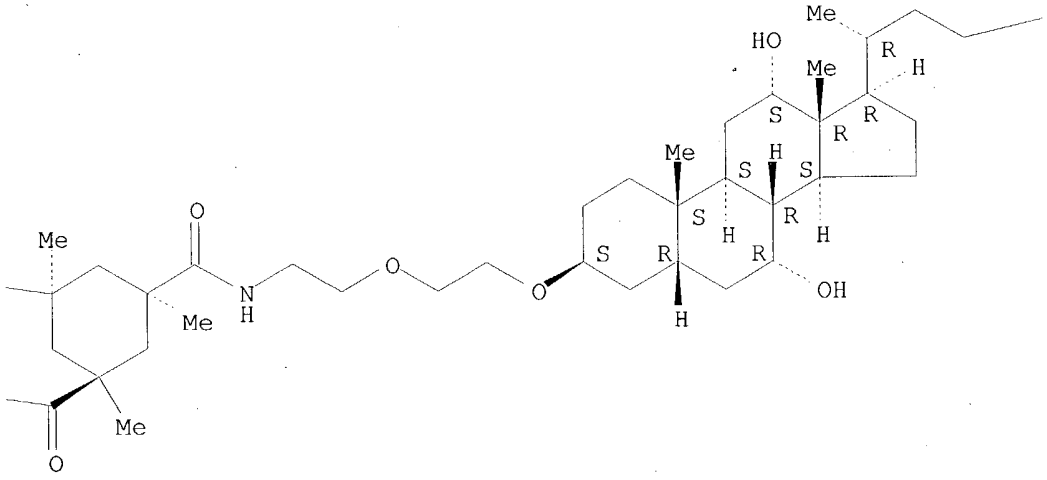

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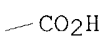

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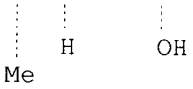

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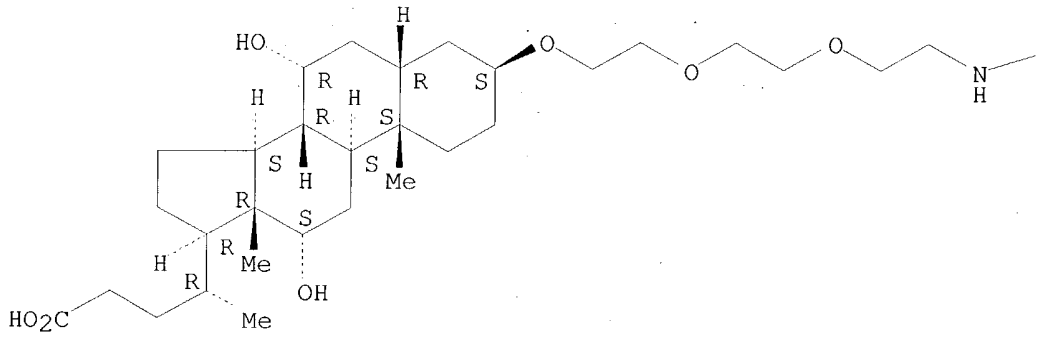
CN Cholan-24-oic acid, 3,3',3''-[(1,3,5-trimethyl-1,3,5-cyclohexanetriyl)tris(carbonylimino-2,1-ethanediyloxy-2,1-ethanediyloxy-2,1-ethanediyloxy)]tris[7,12-dihydroxy-, stereoisomer (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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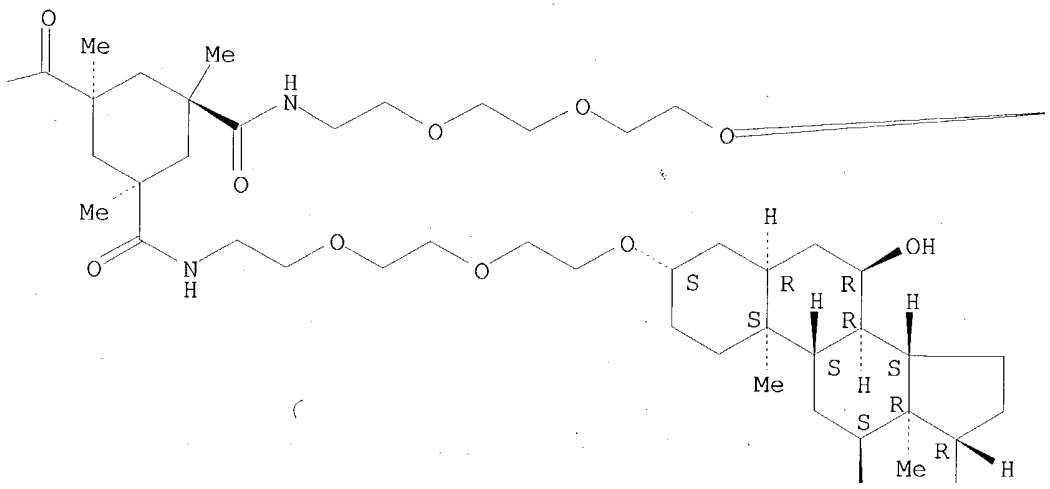

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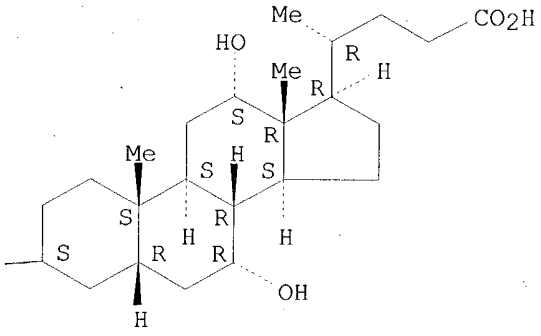

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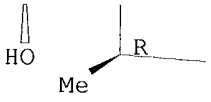

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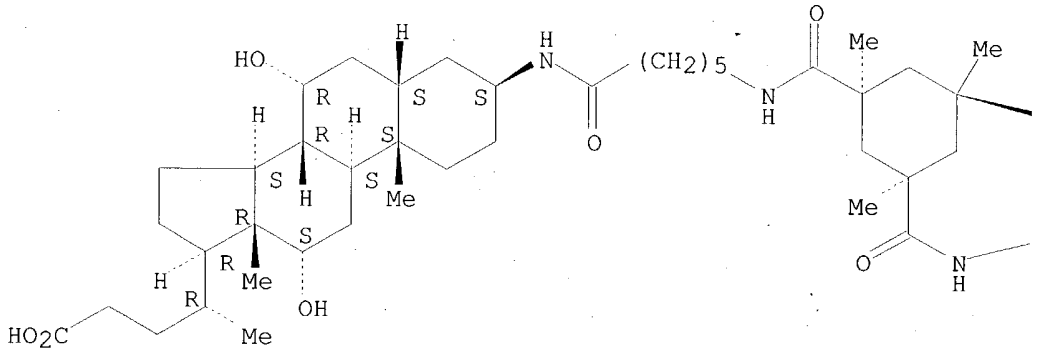
RN 153583-09-6 HCAPLUS
CN Cholan-24-oic acid, 3,3',3''-[(1,3,5-trimethyl-1,3,5-cyclohexanetriyl)tris[carbonylimino(1-oxo-6,1-hexanediyl)imino]]tris[7,12-dihydroxy-, stereoisomer (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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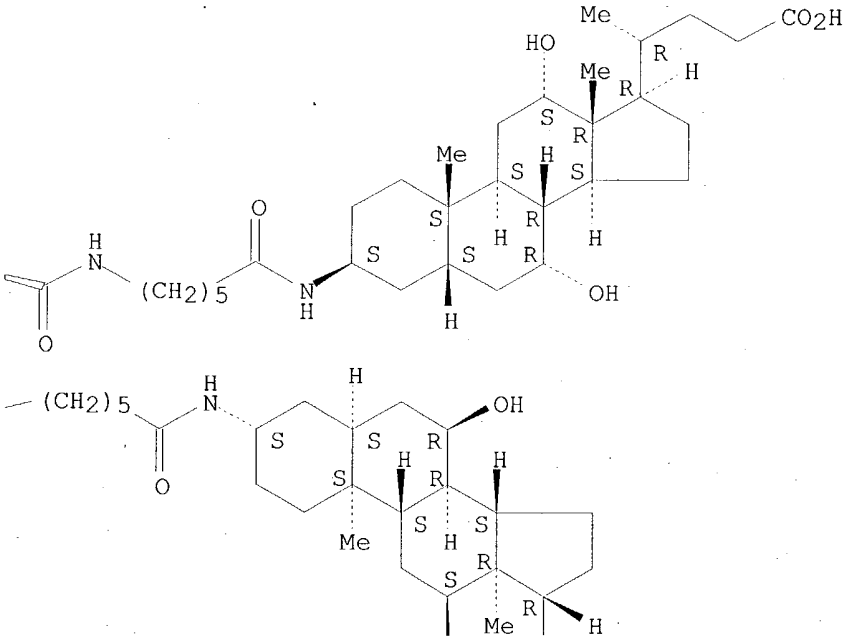
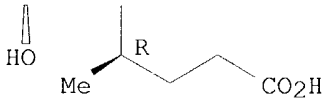


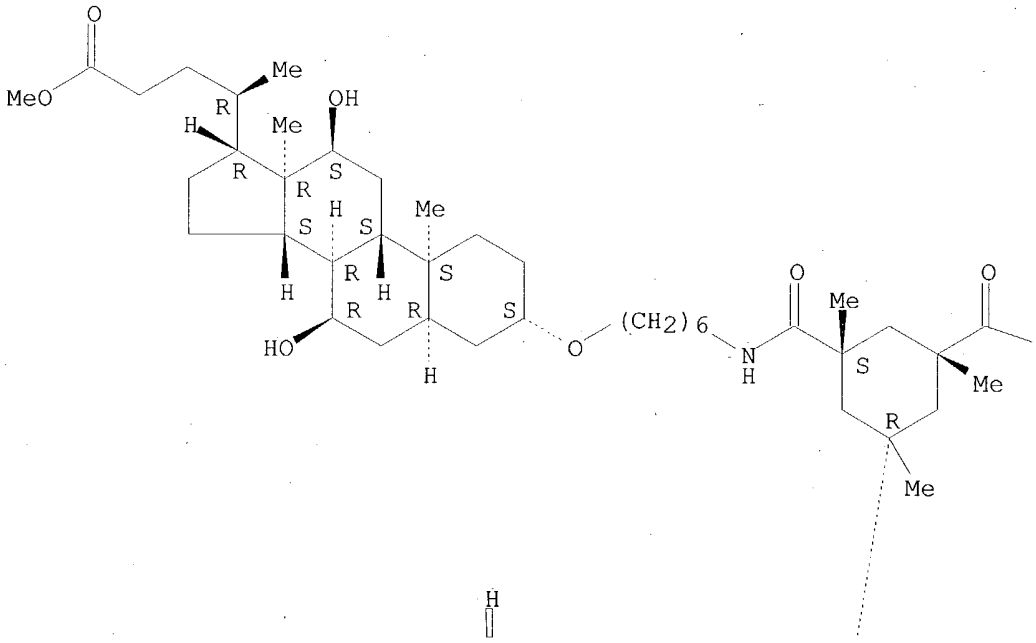
PAGE 2-B



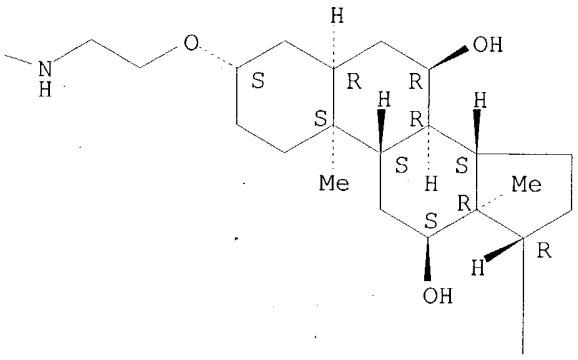
RN 153583-11-0 HCAPLUS
CN Cholan-24-oic acid, 3,3'-[[5-[[[2-[(7,12-dihydroxy-24-methoxy-24-oxocholan-3-yl)oxy]ethyl]amino]carbonyl]-1,3,5-trimethyl-1,3-cyclohexanediyl]bis(carbonylimino-6,1-hexanediyloxy)]bis[7,12-dihydroxy-, dimethyl ester, stereoisomer (9CI) (CA INDEX NAME)

Absolute stereochemistry.

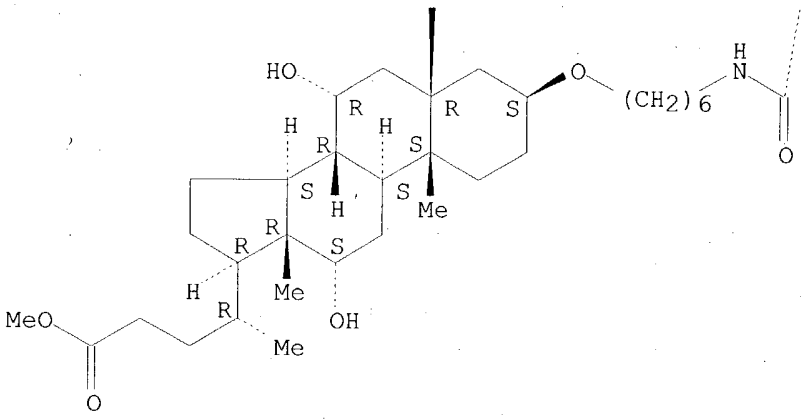
PAGE 1-A



PAGE 1-B



PAGE 2-A



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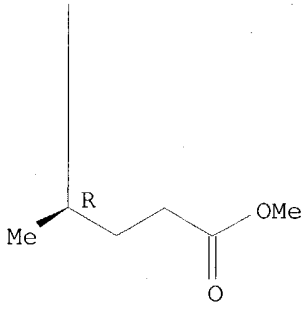
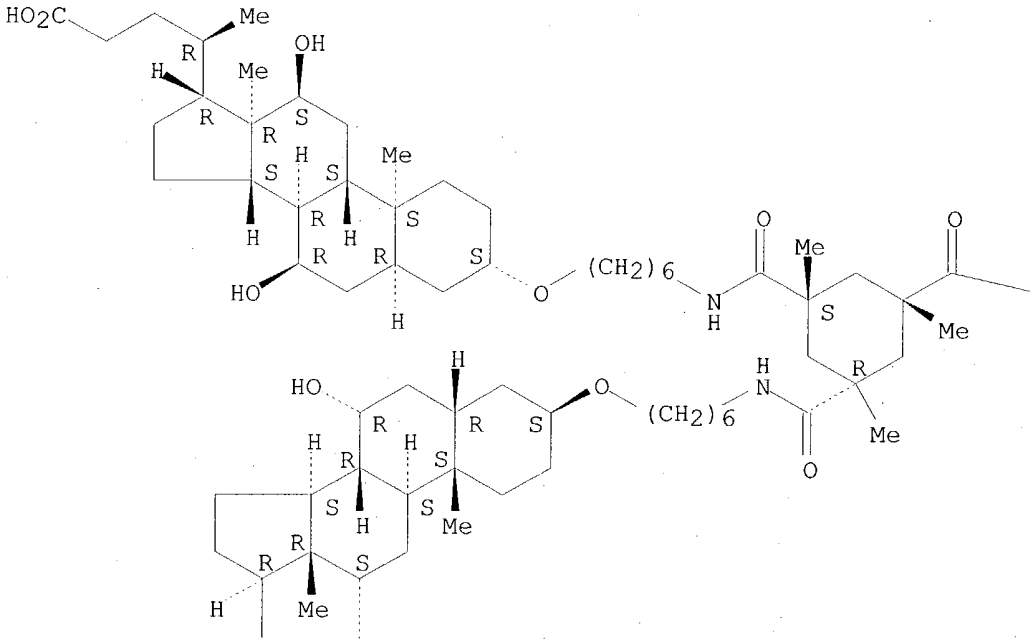


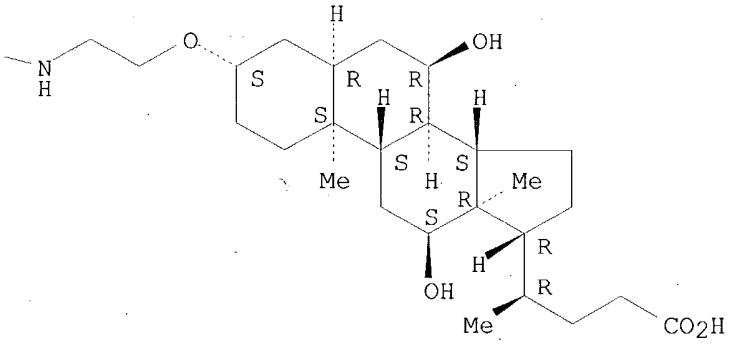
RN 153583-12-1 HCAPLUS
CN Cholan-24-oic acid, 3,3'-[[5-[[[2-[(23-carboxy-7,12-dihydroxy-24-norcholan-3-yl)oxy]ethyl]amino]carbonyl]-1,3,5-trimethyl-1,3-cyclohexanediyl]bis(carbonylimino-6,1-hexanediyloxy)]bis[7,12-dihydroxy-, stereoisomer (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



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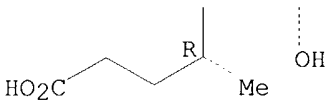
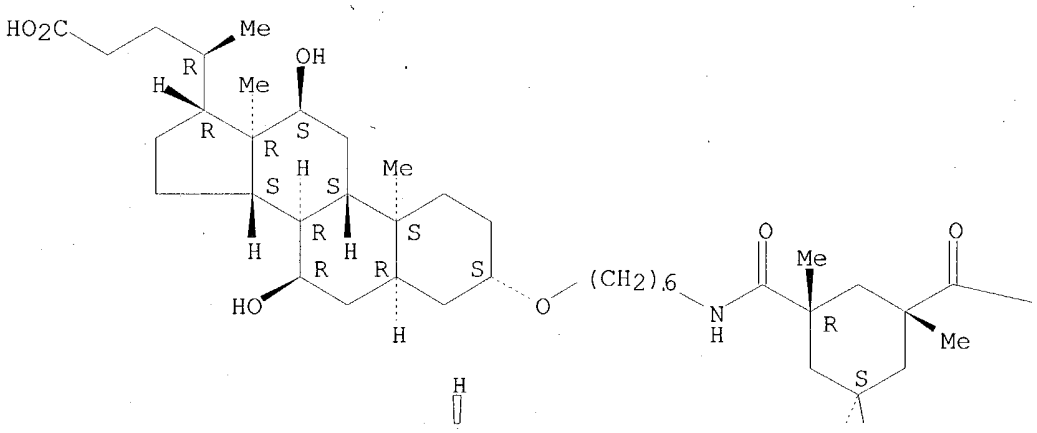


RN 153583-13-2 HCAPLUS
CN Cholan-24-oic acid, 3,3'-[[5-[[[6-[[24-[[6-[(23-carboxy-7,12-dihydroxy-24-norcholan-3-yl)oxy]hexyl]amino]-7,12-dihydroxy-24-oxocholan-3-yl]oxy]hexyl]amino]carbonyl]-1,3,5-trimethyl-1,3-cyclohexanediyl]bis(carbonylimino-6,1-hexanediyloxy)]bis[7,12-dihydroxy-, stereoisomer (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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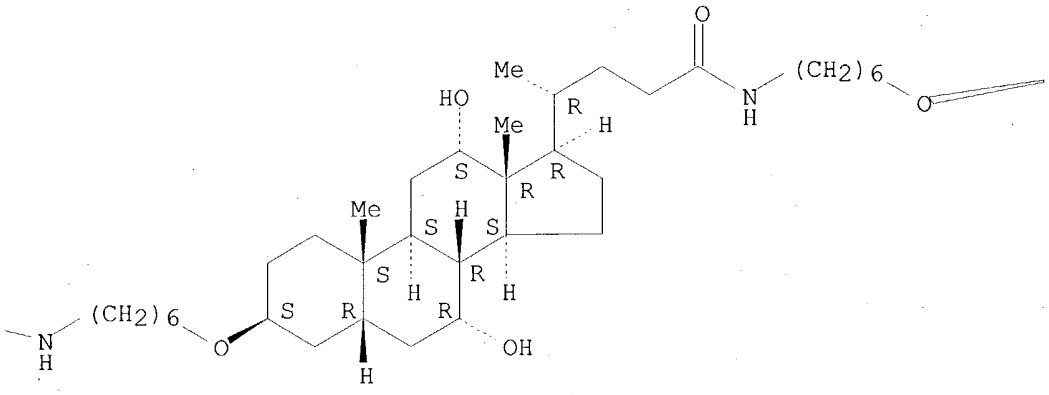
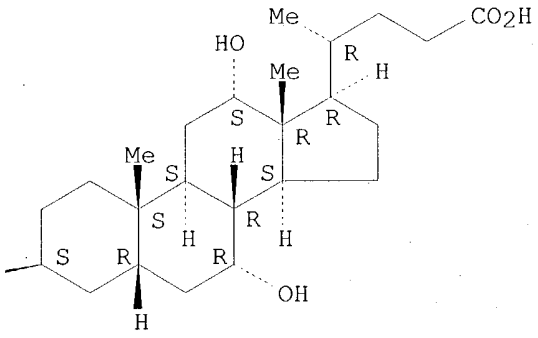


PAGE 1-C



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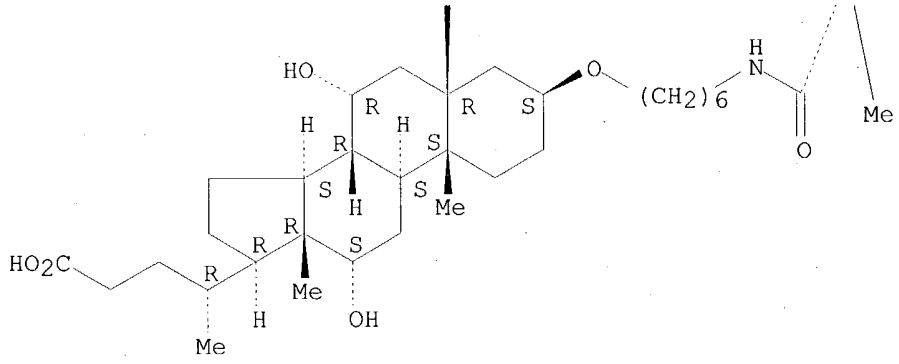
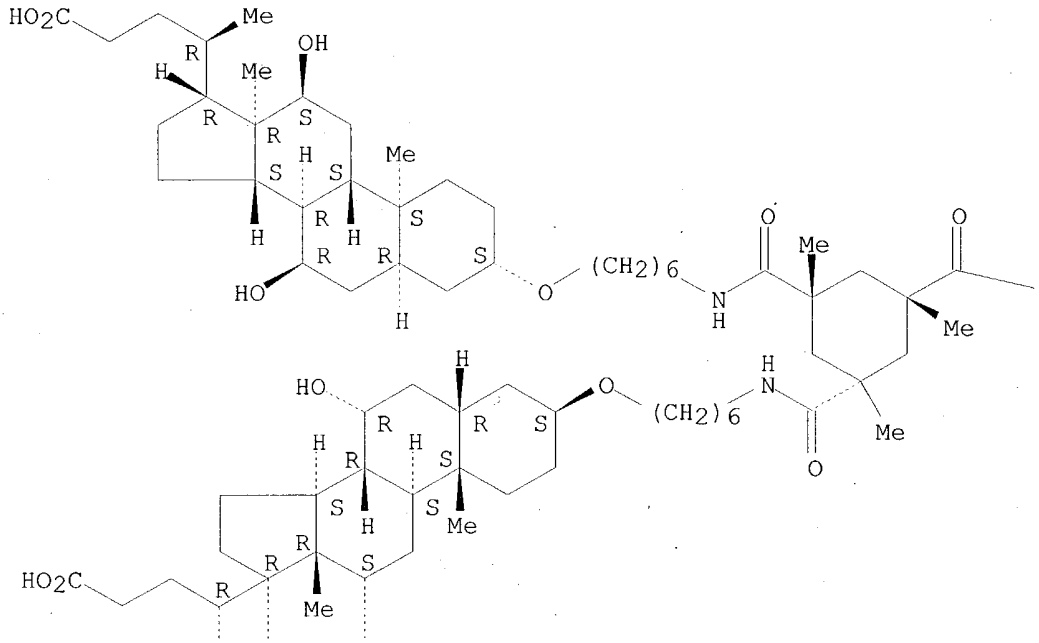


RN 153665-88-4 HCAPLUS
CN Cholan-24-oic acid, 3,3',3''-[(1,3,5-trimethyl-1,3,5-cyclohexanetriyl)tris(carbonylimino-6,1-hexanediyloxy)]tris[7,12-dihydroxy-

, trisodium salt, stereoisomer (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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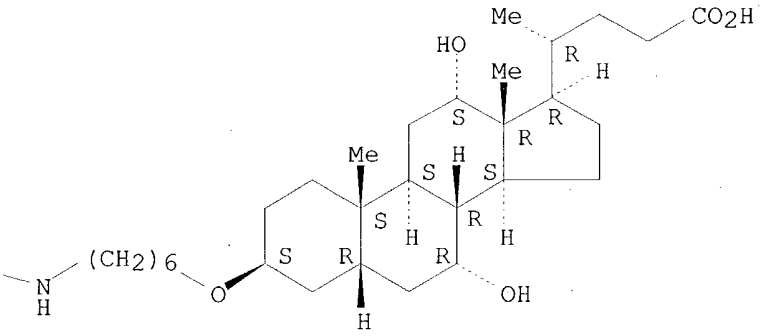

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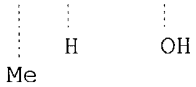


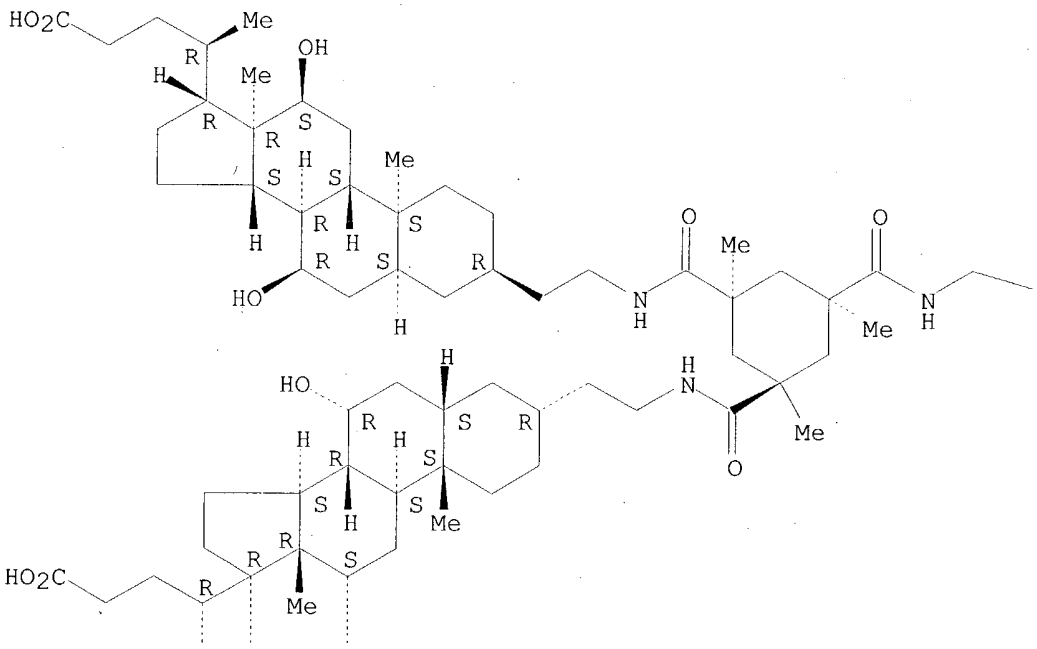
●3 Na

RN 153665-89-5 HCAPLUS
CN Cholan-24-oic acid, 3,3',3''-[(1,3,5-trimethyl-1,3,5-

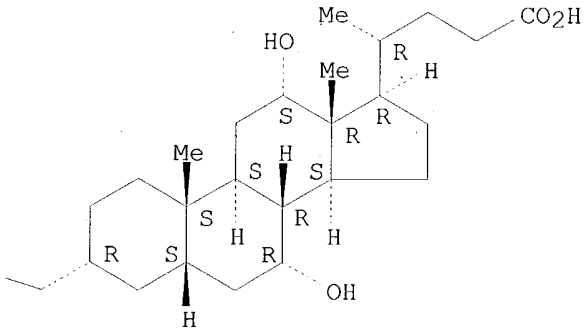
cyclohexanetriyl)tris(carbonylimino-2,1-ethanediyl)]tris[7,12-dihydroxy-, stereoisomer (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



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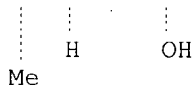
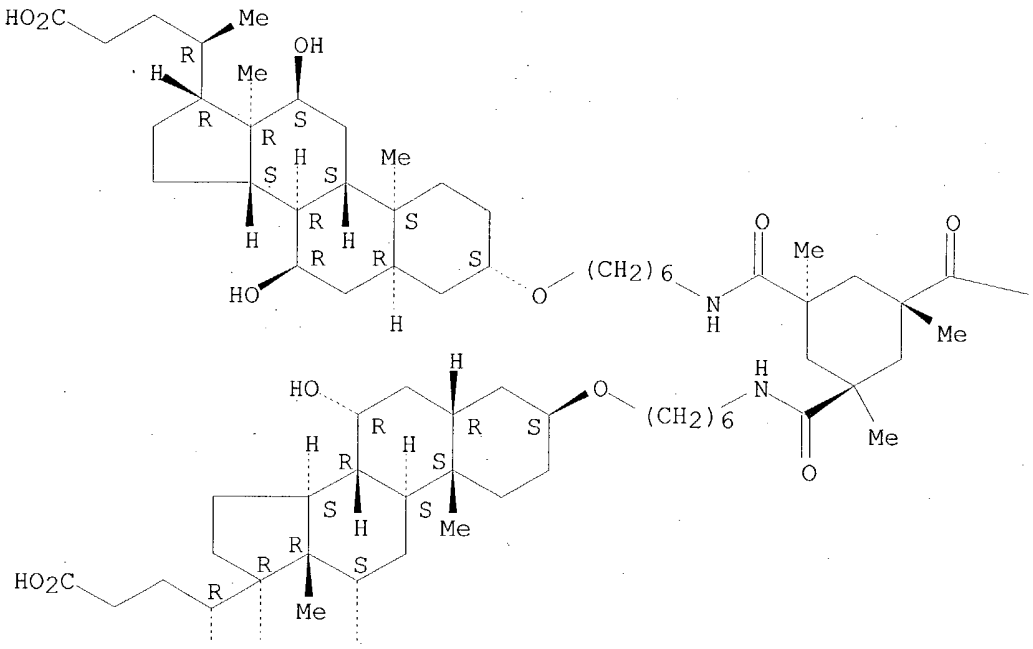


RN 153665-90-8 HCAPLUS
CN Cholan-24-oic acid, 3,3',3''-[(1,3,5-trimethyl-1,3,5-cyclohexanetriyl)tris(carbonylimino-6,1-hexanediyloxy)]tris[7,12-dihydroxy-, stereoisomer (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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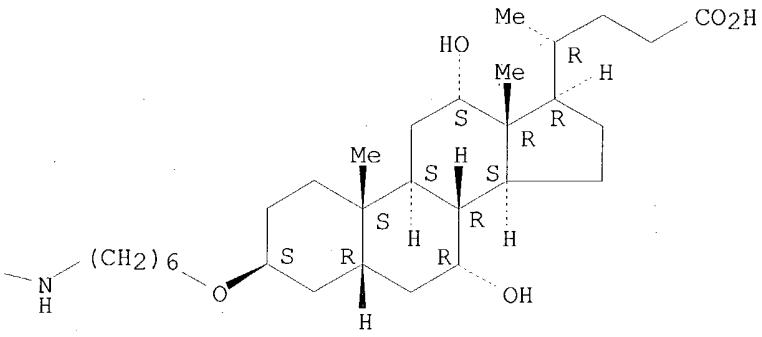

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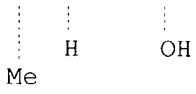
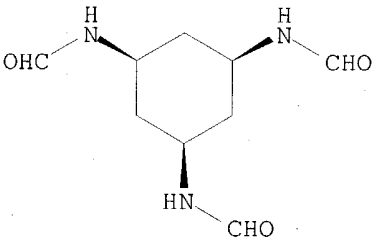


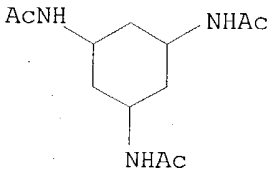
L27 ANSWER 55 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1980:614624 HCAPLUS
DOCUMENT NUMBER: 93:214624
TITLE: Synthesis and metal carbonyl complexes of cis,cis-1,3,5-triisocyanocyclohexane, an unusual tridentate ligand
AUTHOR(S): Michelin, Rino A.; Angelici, Robert J.
CORPORATE SOURCE: Dep. Chem., Iowa State Univ., Ames, IA, 50011, USA

SOURCE: Inorganic Chemistry (1980), 19(12), 3853-6
CODEN: INOCAJ; ISSN: 0020-1669
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The prepn. of cis,cis-1,3,5-triisocyanocyclohexane (L) by dehydration of cis,cis-1,3,5-triformamidocyclohexane with SOCl2 and the reactions of L with transition metal carbonyl complexes to give .mu.3-L[M(CO)5]3 (M = Cr, W) and .mu.3-L[Fe(CO)4]3 are described. The complexes were characterized by chem. anal. and IR and 1H and 13C NMR spectra.
IT **75030-35-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and dehydration of, with thionyl chloride)
RN 75030-35-2 HCAPLUS
CN Formamide, N,N',N''-1,3,5-cyclohexanetriyltris-, (1.alpha.,3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

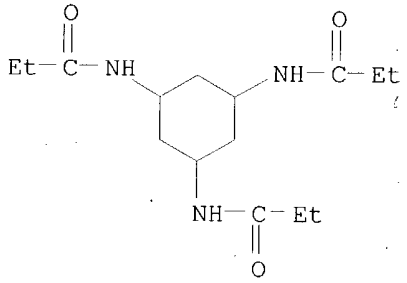
Relative stereochemistry.



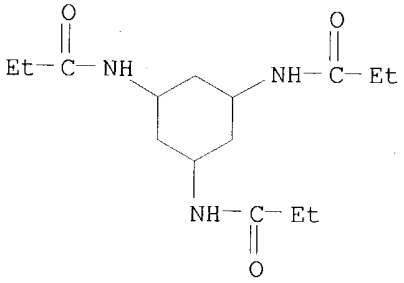
L27 ANSWER 56 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1970:55386 HCAPLUS
DOCUMENT NUMBER: 72:55386
TITLE: Compounds with urotropine structure. XLV. Cyclizations starting from 1,3,5-triaminocyclohexane
AUTHOR(S): Stetter, Hermann; Theisen, Dieter; Steffens, Gerd J.
CORPORATE SOURCE: Inst. Org. Chem., Tech. Hochsch. Aachen, Aachen, Fed. Rep. Ger.
SOURCE: Chemische Berichte (1970), 103(1), 200-4
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 72:55386
GI For diagram(s), see printed CA Issue.
AB 1,3,5-(O2N)3C6H3 was hydrogenated on Pd/C in AcOEt and R2O to 1,3,5-(RNH)3C6H3 which on further hydrogenation gave .apprx.20% trans and 80% cis isomers of cyclohexanes (I) [where R = Ac or EtCO (Ia)]. trans-Ia was converted with HC(OEt)3 at 265.degree. to the 2,4,10-triazaadamantane (II) (R = EtCO). This on sapon. gave pure cis-I (R = H). Both cis- and trans-I (R = PhSO2), obtained from I (R = H) with PhSO2Cl, and CH(OEt)3 were similarly converted to II (R = PhSO2). However, PhSO2NHMe and CH(OEt)3 gave (PhSO2NMe)2CH(OEt).
IT **26159-20-6P 26159-21-7P 26159-22-8P 26251-47-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 26159-20-6 HCAPLUS
CN Acetamide, N,N',N''-1,3,5-cyclohexanetriyltris-, cis-1,3, cis-1,5- (8CI) (CA INDEX NAME)



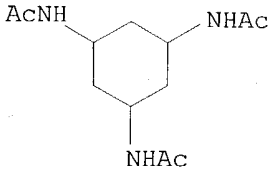
RN 26159-21-7 HCAPLUS
CN Propionamide, N,N',N''-1,3,5-cyclohexanetriyltris-, cis, cis- (8CI) (CA INDEX NAME)



RN 26159-22-8 HCAPLUS
CN Propionamide, N,N',N''-1,3,5-cyclohexanetriyltris-, stereoisomer (8CI) (CA INDEX NAME)



RN 26251-47-8 HCAPLUS
CN Acetamide, N,N',N''-1,3,5-cyclohexanetriyltris-, stereoisomer (8CI) (CA INDEX NAME)



L27 ANSWER 57 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1955:69098 HCAPLUS
DOCUMENT NUMBER: 49:69098
ORIGINAL REFERENCE NO.: 49:13242d-i,13243a-h
TITLE: Attempted syntheses of nitrogen analogs of adamantane
AUTHOR(S): Newman, Melvin S.; Lowrie, Harman S.

CORPORATE SOURCE: Ohio State Univ., Columbus
SOURCE: Journal of the American Chemical Society (1954), 76, 4598-600
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

AB Attempts to prep. N analogs of adamantane from 1,3,5-trisubstituted cyclohexanes failed. A no. of these cyclohexanes were related in configuration, postulated to be cis. 1,3,5-C6H3(CO2Me)3, white needles, m. 145-6.degree. (from MeOH), reduced and distd. gave tri-Me 1,3,5-cyclohexanetricarboxylate (I), semisolid cryst. mixt. of isomers, which was recrystd. 3 times from Et2O at -70.degree.; in the best of several runs, 33.3 g. mixt. gave 20.6 g., solid I, m. 48.0-9.0.degree. (all m. ps. are cor.); addnl. crops could be obtained from the mother liquors. Solid I (30.0 g.) reduced with LiAlH4 slurried in Et2O, the mixt. acidified with dil. H2SO4, satd. with Na2SO4, and extd. continuously 12 days with Et2O, the ext. dild. with MeOH, the soln. passed through Al2O3 to remove traces of acid, and the solvents removed gave 14.6 g. oily yellow solid, which recrystd. 3 times from Me2CO gave 1,3,5-cyclohexanetrimethanol (II), white rods, m. 101.0-2.0.degree.. Isomeric mixt. (43.8 g.) of I reduced in the same way gave 32.5 g. oily solid which recrystd. from Me2CO gave 8.4 g. II, m. 97-100.degree.; the mother liquor evapd. to dryness, the residual oil refluxed with dil. aq. NaOH, and the soln. satd. with Na2SO4 and extd. with Et2O in the usual manner yielded 10.6 g. II, m. 95-100.degree.. II (2.10 g.) in dry pyridine treated 3 hrs. at -5 to 0.degree. with MeSO2Cl, the mixt. worked up in the cold, the resulting yellow solid dissolved in Me2CO, the soln. passed through Norit A and the solvent removed with air gave 4.4 g. trimethanesulfonate (III) of II, white crystals, m. 125.5-6.5.degree. (recrystd. twice from Me2CO-Et2O, m. 126.8-7.4.degree.). Crude III (35 g.), m. 108-18.degree., shaken overnight in a steel bomb with 500 cc. dioxane and 0.6 mole dry NH3, the mixt. heated slowly to 85.degree. for 24 hrs., cooled, treated with 0.2 mole NH3, heated 24 hrs. at 95.degree., cooled, poured into dil. H2SO4, steam distd. to remove the dioxane, made strongly basic, and again steam distd., the distillate collected in dil. HCl until it was no longer basic, the resulting soln. evapd., the yellow-white solid residue dried and extd. once with Me2CO to remove the yellow color and 3 times with CHCl3, the CHCl3 ext. evapd., and the white powdery residue (0.42 g., 2.8%) recrystd. from EtOH-PhMe gave a compd. C9H15N (IV).HCl, white crystals, insol. in Me2CO, but readily sol. in CHCl3. IV.HCl treated 12 hrs. at 95.degree. with aq. HNO2 was recovered unchanged. IV.HCl sublimed at 180-200.degree. before melting in an open tube and melted above 400.degree. in a sealed tube. Alk. aq. KMnO4 was immediately discolored by the addn. of 0.10 g. IV.HCl in base; the soln. treated with KMnO4 until the color persisted, refluxed 1 hr., and distd. gave less than 5 mg. white powder identified as NH4Cl. IV.HCl in CHCl3 treated dropwise with Br in CCl4 until the Br color persisted, the solvents removed with air, the orange solid residue dissolved in abs. EtOH, the soln. dild. with ligroine (b. 90-7.degree.), and the yellow ppt. washed with a small amt. of Me2CO and recrystd. from boiling Me2CO deposited 2 crystal forms which were sepd. manually, washed with cold Me2CO, and dried to give 20 mg. compd. C9H15Br2N, long needles, fairly sol. in Me2CO; and 15 mg. IV.HBr, small cubes, rather insol. in Me2CO. A small amt. of IV.HCl dissolved in HBr and the soln. evapd. gave IV.HBr. I (20.5 g.) refluxed 2-3 hrs. with dil. NaOH, the soln. concd., acidified with H2SO4, satd. with Na2SO4, and extd. continuously 12 hrs. with Et2O, and the ext. evapd. gave 18.0 g. 1,3,5-cyclohexanetricarboxylic acid-1.5H2O (V.1.5-H2O), white powdery solid, m. 208-13.degree., which gave, recrystn. 3 times from Me2CO-C6H6, V, white needles, m. 215-18.degree.. V (1.30 g.) treated with CH2N2 gave 1.22 g. solid, m. 43-7.degree., which distd. and recrystd. from Et2O at -70.degree. gave I, fine needles, m. 48-9.degree.. V treated with SOCl2, the resulting acid chloride dissolved in C6H6, the soln. added to 28%

NH4OH, the aq. layer cooled and filtered, and the filter residue recrystd. twice from H2O yielded 1,3,5-cyclohexanetricarboxamide (VI), white crystals, m. 287.5-8.5.degree. (decompn.) with softening at 283.5.degree.. VI (1.24 g.) sublimed during 6 hrs. at 285.degree. gave 0.81 g. (78%) sublimate (collected in several fractions), m. between 210 and 240.degree. in 20.degree. ranges; this sublimate boiled with EtOH in which it was rather insol., the EtOH removed, and the residue recrystd. twice from Me2CO gave VII (R = CN), white crystals, m. 239-43.degree. with darkening after softening at 230-1.degree.. V (1.3 g.) in 5 cc. 28% NH4OH evapd. to dryness, the residue pyrolyzed at 270-300.degree., and the white solid sublimate dried in vacuo gave 0.90 g. material, m. 230-50.degree. (decompn.) with softening at 190-220.degree., which recrystd. twice from EtOH-PhMe yielded a compd. C9H11NO4 (VIII), white poorly formed crystals, m. 244-7.degree. (decompn.) with softening at 240-4.degree.. V (6.1 g.) gave similarly 4.2 g. material which was sublimed and collected in fractions; 1 fraction resublimed at 195.degree. and 0.1 mm. gave white powdery crystals, m. 215-33.degree. (decompn.) with softening at 204.degree.; another fraction recrystd. twice from EtOH-PhMe and then sublimed at 195.degree. and 0.1 mm. gave a white powder, m. 227-54.degree. (decompn.) with softening at 223.degree.. The various fractions of VIII, which was a mixt. of IX and VII (R = CO2H), showed initially neutral equivs. of 280-300 which dropped to a final value of 108-14 when excess base was added. A portion of the material upon which the neutral equiv. had been taken boiled with dil. aq. NaOH, the mixt. acidified with HCl and evapd. to dryness, the residue extd. with Me2CO, the ext. evapd., and the residue recrystd. from EtOH-PhMe gave V, white needles, m. 211-15.degree.. V treated with CH2N2 gave I, clear needles, m. 48-9.degree.. V (10.8 g.) treated with NH4OH, the mixt. evapd., and the residue pyrolyzed gave 6.6 g. product having the same m.p. range and infrared spectrum as the sublimates of VIII; a 3-g. sample let stand 2 days with SOCl2, the mixt. refluxed a short time and evapd. in vacuo, and the residue sublimed at 35 mm. gave 0.9 g. VII (R = COCl) (X), white needles, m. 170-80.degree. (rapid heating). X (0.3 g.) in CHCl3 previously satd. with NH3 let stand 1 hr., filtered, and evapd., and the residue sublimed and then recrystd. from Me2CO-C6H6 gave 0.05 g. tan crystals, m. 260-5.degree.; the mother liquor evapd. gave VII (R = CN), white crystals, m. 207-20.degree..

IT **99063-92-0**, 1,3,5-Cyclohexanetricarboxamide
(prepn. of)

RN 99063-92-0 HCAPLUS

CN 1,3,5-Cyclohexanetricarboxamide (6CI, 9CI) (CA INDEX NAME)